Global Leaders in Slurry Systems Engineering

Established in 1991 in Cape Town, Paterson & Cooke is a recognised leader in the design of slurry pipeline systems and associated technologies. Engineering and test services are offered from our worldwide network of offices for all aspects of slurry handling projects.

Our service capability includes the following key areas of expertise:

- Long distance pipeline engineering, from conceptual to detailed engineering design, construction assistance, commissioning and operator training.
- Conventional, thickened and paste tailings systems engineering.
- Mine backfill, hydraulic and paste backfill material selection and strength testing, design and engineering of backfill preparation plants and piping systems.
- Process engineering expertise covering a wide range of mineral processing technologies including comminution, classification, beneficiation and solid-liquid separation.
- Specialist engineering services including CFD analysis, pipe stress analysis, transient flow simulation and long distance pipeline control systems.
- Field services upgrades, retrofits and process optimisation on existing operations.
- Pilot plant facility design, turnkey supply and on-site operation.
- Slurry laboratory services providing a full range of test capabilities for mineral processing, tailings management, mine backfill and slurry pipeline applications.
- Marine and coastal dredging and mining systems.
- Specialised training courses.

South African Offices

CAPE TOWN
Paterson & Cooke Consulting Engineers (Pty) Ltd
Sunrise Park, Prestige Drive, Sunrise Circle, Ndabeni, 7405, Cape Town, South Africa
PO Box 38045, Pinelands, 7430, South Africa
Tel: +27 (0) 21 531 2955 Fax: +27 (0) 86 546 9876
CapeTown@PatersonCooke.com

JOHANNESBURG
Paterson & Cooke Field Services
Unit 19, Norma Jean Square, 244 Jean Avenue, Centurion, 0157, South Africa
Postnet Suite #454, Private Bag X2, Rasilouw, 0109, South Africa
Tel: +27 (0) 86 010 6129 Fax: +27 (0) 86 546 9876
Johannesburg@PatersonCooke.com

Our key strength is the intellect, creativity and commitment of the people who work for Paterson & Cooke.
Virtual Reality and spatial information applications in the mining industry Conference 2015

University of Pretoria
15–16 July 2015

BACKGROUND

Virtual Reality (VR) is a continuously evolving technology where a user interacts with a three-dimensional computer-simulated environment, which the user perceives as comparable to real world objects and events. As computer hardware and software technology have improved, the ease with which interactive simulations can be developed and deployed has improved significantly and lower cost, high-quality development tools have become available. VR applications in education and training have become increasingly popular in the context of effective knowledge transfer. Although VR technology has improved significantly over the last few years, its potential advantages with specific reference to Safety Health and the Environment (SHE) and mine planning and design, are relatively unknown.

Mining technical information is three dimensional. Miners think in pictures of their holes in the ground. Recent advances in open standard spatial data formats have opened up new and highly visual opportunities for integrated information management. Routine reporting and analytical exercises create new levels of insight into mining issues and challenges.

The ability to integrate mining technical data irrespective of source (323 and counting) opens up the possibility of integration with commercial information, access to readily available analytical toolsets and therefore has consequences across the enterprise.

For further information contact:
Conference Co-ordinator, Camielah Jardine
SAIMM, P O Box 61127, Marshalltown 2107
Tel: (011) 834-1273/7
Fax: (011) 833-8156 or (011) 838-5923
E-mail: camielah@saimm.co.za
Website: http://www.saimm.co.za

Conference Announcement
OFFICE BEARERS AND COUNCIL FOR THE
2014/2015 SESSION

Honorary President
Mike Teke
President, Chamber of Mines of South Africa

Honorary Vice-Presidents
Ngoako Ramathodi
Minister of Mineral Resources, South Africa
Rob Davies
Minister of Trade and Industry, South Africa
Naizeli Fandu
Minister of Science and Technology, South Africa

President
J.L. Porter

President Elect
R.T. Jones

Vice- Presidents
C. Musingwini
S. Ndlovu

Immediate Past President
M. Dworzanowski

Honorary Treasurer
C. Musingwini

Ordinary Members on Council
V.G. Duke
M.F. Handley
A.S. Macfarlane
M. Motuku
M. Mthenjane
D.D. Munro
G. Njowa

Past Presidents Serving on Council
N.A. Barcza
R.D. Beck
J.A. Cruise
J.R. Dixon
F.M.G. Egerton
G.V.R. Landman
R.P. Mhoring

Branch Chairmen
DRC
S. Maleba
Johannesburg
I. Ashmole
Namibia
N.M. Namate
Northern Cape
C. van Wyk
Pretoria
N. Naude
Western Cape
C. Dorfling
Zambia
D. Muma
Zimbabwe
S. Ndyamba
Zululand
C.W. Mienie

Corresponding Members of Council
Australia: I.J. Corrans, R.J. Dippenaar, A. Croll, C. Workman-Davies
Austria: H. Wagner
Botswana: S.D. Williams
United Kingdom: J.J. Cilliers, N.A. Barcza
USA: J.M.M. Rendu, P.C. Pistorius

PAST PRESIDENTS

*Deceased
* W. Bettel (1894–1895)
* A.F. Crosse (1895–1896)
* W.R. Feldmann (1896–1897)
* C. Butters (1897–1898)
* J. Leocy (1898–1899)
* J.R. Williams (1899–1900)
* S.H. Pearce (1900–1902)
* W.A. Caldcott (1904–1905)
* W. Cullen (1905–1906)
* E.H. Johnson (1906–1907)
* J. Yates (1907–1908)
* R.G. Bevington (1908–1909)
* A. McCa. Johnston (1909–1910)
* J. Moir (1910–1911)
* C.B. Saner (1911–1912)
* W.R. Dowling (1912–1913)
* A. Richardson (1913–1914)
* G.H. Stanley (1914–1915)
* J.E. Thomas (1915–1916)
* J.A. Wilkinson (1916–1917)
* G. Hlack-Smith (1917–1918)
* H.S. Meyer (1918–1919)
* J. Gray (1919–1920)
* J. Chilton (1920–1921)
* F. Wartenweiler (1921–1922)
* G.A. Waermeier (1922–1923)
* F.W. Watson (1923–1924)
* C.J. Gray (1924–1925)
* H.A. White (1925–1926)
* H.R. Adam (1926–1927)
* Sir Robert Kotze (1927–1928)
* J.A. Woodburn (1928–1929)
* H. Pirow (1929–1930)
* J. Henderson (1930–1931)
* A. King (1931–1932)
* V. Nimmo-Dewar (1932–1933)
* P.N. Latgean (1933–1934)
* E.C. Ranson (1934–1935)
* P.R. Jochens (1935–1936)
* G.H. Stanley (1936–1937)
* R.P. Plewman (1937–1938)
* T.K. Prentice (1938–1939)
* J. Loevy (1939–1940)
* P.E. Hall (1940–1941)
* R.S.G. Stokes (1941–1942)
* A. Clemens (1942–1943)
* M. Falcon (1943–1944)
* C. Biccard Jeppe (1944–1945)
* J.T. McIntyre (1945–1946)
* P.J. Louis Bok (1946–1947)
* J. Chilton (1947–1948)
* W.J. van Rensburg (1947–1948)
* A.A.B. Douglas (1948–1949)
* H.E.A. Joseph (1949–1950)
* P.N. Lategan (1950–1951)
* W.E. Gooday (1951–1952)
* J.P. Hoffman (1952–1953)
* H.R. Adam (1953–1954)
* E.H. Johnson (1954–1955)
* Wm. Bleloch (1955–1956)
* H. Briten (1956–1956)
* H. Simon (1957–1958)
* M. Barcza (1958–1959)
* B.L. Adamson (1959–1960)
* D.G. Findlay (1960–1961)
* J. de V. Lambrechts (1962–1963)
* D.M. Jamieson (1964–1965)
* H.E. Cross (1965–1966)
* P. Lambooy (1967–1968)
* V.C. Robinson (1970–1971)
* J.P. Hugo (1972–1973)
* P.W.J. van Rensburg (1973–1974)
* M.D.G. Salamon (1976–1977)
* M.G. Amrose (1978–1979)
* J.D. Austin (1984–1985)
* H. Wagner (1986–1987)
* N.A. Barcza (1996–1997)
* M.H. Rogers (1999–2000)
* A.M. Garbers-Craig (2008–2009)
* J.C. Ngoma (2009–2010)
* G.V.R. Landman (2010–2011)
* J.N. van der Merwe (2011–2012)
* G.L. Smith (2012–2013)

Honorary Legal Advisers
Van Hulsteyns Attorneys

Auditors
Messrs R.H. Kitching

Secretaries
The Southern African Institute of Mining and Metallurgy
Fifth Floor, Chamber of Mines Building
5 Hollard Street, Johannesburg 2001
P.O. Box 61127, Marshalltown 2107
Telephone (011) 834-1273/7
Fax (011) 838-5923 or (011) 833-8156
E-mail: journal@saimm.co.za

The Journal of The Southern African Institute of Mining and Metallurgy
Contents

Journal Comment ........................................ iv

President’s Corner ....................................... vii

Spotlight: SANCOT News ............................... vi

The SAIMM Young Professionals’ Council (SAIMM-YPC) by T. Mmola ........................................ v

PLATINUM CONFERENCE PAPERS

Predicting the probability of Iron-Rich Ultramafic Pegmatite (IRUP) in the Merensky Reef at Lonmin’s Karee Mine by D. Hoffmann and S. Plumb ........................................ 465

Tough choices facing the South African mining industry by A. Lane, J. Güzek, and W. van Antwerpen ........................................ 471

Crush pillar support – designing for controlled pillar failure by M. du Plessis and D.F. Malan ........................................ 481

The application of pumpable emulsions in narrow-reef stopping by S.P. Pearton ........................................ 489

Corrosion resistance of laser-cladded 304L stainless steel enriched with ruthenium additions exposed to sulphuric acid and sodium chloride media by J. van der Merwe and D. Tharandt ........................................ 499

Fire and brimstone: The roasting of a Merensky PGM concentrate by R.I. Rambiyana, P. den Hoed, and A.M. Garbers-Craig ........................................ 507

Strategic and tactical requirements of a mining long-term plan by B.J. Kloppers, C.J. Horn, and J.V.Z. Visser ........................................ 515

GENERAL PAPERS

Integration of imprecise and biased data into mineral resource estimates by A. Cornah and E Machaka ........................................ 523

Stochastic simulation for budget prediction for large surface mines in the South African mining industry by J. Hager, V.S.S. Yadavalli, and R. Webber-Youngman ........................................ 531

Q-coda estimation in the Kaapvaal Craton by D.J. Birch, A. Cichowicz, and D. Grobbelaar ........................................ 541

Geometallurgical model of a copper sulphide mine for long-term planning by G. Compan, E. Pizarro, and A. Videla ........................................ 549

Introduction to the production of clean steel by J.D. Steenkamp and L. du Preez ........................................ 557

International Advisory Board
R. Dimitrakopoulos, McGill University, Canada
D. Dreisinger, University of British Columbia, Canada
E. Esterhuizen, NSWHS Research Organization, USA
H. Mitas, McGill University, Canada
M.J. Nicol, Murdoch University, Australia
E. Topal, Curtin University, Australia
Pyrometallurgical operations are essentially concerned with the high-temperature processing of materials. These chemical processes can be extremely complex, involving reactions between gas, solids, liquid slag, and liquid metal (and sometimes other phases as well). In addition to the chemistry, consideration must also be given to the energy supply, containment, and flow of the various streams. Pyrometallurgical processes must be evaluated at many stages during their development and design, and when operating changes are introduced. Because experimental work in pyrometallurgy is expensive, a system should be characterized as thoroughly as possible before experimental work is undertaken. Computer simulation allows the requirements of a particular process to be determined quickly and reliably.

Pyrometallurgy is at least 6000 years old, with the oldest known smelters being used for the production of copper in the Middle East. Mathematical modelling, at least in its simplest form, is much older than this. The oldest known mathematical artefact is considered to be the Lebombo bone – a 35 000-year-old baboon fibula discovered in a cave in the Lebombo Mountains in Swaziland in the 1970s – that has a series of 29 notches that were deliberately cut to help to calculate numbers and perhaps also measure the passage of time. The abacus dates from as early as 2400 BC in Babylon, and was also found in China, Egypt, Greece, and Rome, and used by the Aztecs.

The earliest recognisable computers were the Mark I (1944) and Mark II (1945) developed at Harvard University. These electromagnetic computers are seen as the first universal calculators (even though they lacked branching) and operated at three calculations per second. The first electronic general-purpose computer, ENIAC (Electronic Numerical Integrator And Computer) was built in 1946 at the University of Pennsylvania. ENIAC could do simple addition or subtraction of two ten-digit numbers at the rate of 5000 per second, or could do 357 multiplications per second. ENIAC weighed 27 tons, measured 2.4 m × 0.9 m × 30 m, and consumed 150 kW of power. A rather daring prediction was made in the March 1949 issue of Popular Mechanics: ‘Where a calculator on the ENIAC is equipped with 18,000 vacuum tubes and weighs 30 tons, computers in the future may have only 1,000 vacuum tubes and perhaps weigh 1½ tons.’

In my own lifetime, I progressed from using log tables, then a slide rule, to an early scientific calculator in high school. At university, I started programming in Fortran on a mainframe computer that used punched cards (until the late 1970s). I then used a programmable calculator with less than one kilobyte of memory to design heat exchangers (an oddly named piece of equipment: even if there was a caloric-like substance called ‘heat’, it certainly isn’t exchanged) and cyclones. When I started work, early chemical equilibrium calculations were carried out (slowly and expansively) via a Saponet satellite link to the F*A*C*T thermodynamic database (the predecessor of FactSage) hosted on a mainframe computer at McGill University in Montreal. At that time, calculations were limited in the number of elements that could be accommodated, so the time was ripe for a desktop computer program that could be applied to more complex systems. Pyrosim computer software for the steady-state sequential-modular simulation of pyrometallurgical processes was initially developed at Mintek in 1985 on a 64 kB Apple II computer (1 MHz), and was presented at the APCOM 87 conference in 1987. Pyrosim moved to an MS-DOS version in 1988 when it was first used in industry. This software was originally developed to simulate various process routes for the production of raw stainless steel, but the structure was kept general enough to allow it to be used to calculate predictive steady-state mass and energy balances for a very wide range of processes. Pyrosim thermodynamic modelling software was eventually installed at 95 sites in 22 countries on 6 continents.

Desktop computing improved rapidly, with a roughly 1500-fold increase in speed and storage capacity, from the Apple II to a fast Pentium processor. A typical Pyrosim simulation would have taken over an hour on an Apple II, but just over three seconds on a 33 MHz i486 computer (1200 times faster). A study of
practical desktop supercomputing was carried out in 1993, using a real-world benchmark, written in ‘C’, to solve a finite-volume energy-transfer problem in two-dimensional cylindrical geometry, using the TriDiagonal Matrix Algorithm. The chosen reference computer was a 50 MHz i486 computer (nominally rated at 30 MIPS, or 30 million instructions per second). At that time, the Pentium processor (rated at 100 MIPS) was not yet commercially available. Using this practical test, it was found that the i486-50 was 80 times faster than the original IBM PC (4.77 MHz with 8087 coprocessor), and the well-established Cray 2 supercomputer was in turn 5.25 times as fast as the i486-50. This indicated that the Cray was only about twice as fast as a Pentium for this type of problem. The Cray 2 was rated at 1600 MFlop/s (million floating-point operations per second). Since that time, the computing speed of the world’s fastest supercomputer has increased exponentially, from about 124 GFlop/s (124 x 10^9) in 1994 to about 34 PFlop/s (34 x 10^15) in 2014. A typical personal computer in 2014 was able to run at about 500 GFlop/s – much faster than the world’s fastest supercomputer from 1994.

If we assume that computer power will continue to increase in the way it has done for the past twenty years, it is interesting to consider what might become possible in years to come. For example, a fully resolved model of an industrial-scale electric arc (say 50 kA over about 0.5 m) is expected to require over 200 PFlop/s (about half a million times that of the computing power of today’s personal computers). At current growth predictions, this should be achieved on the world’s fastest computer in 2017, on the 500th fastest computer in 2024, and on the desktop in 2037.

This edition of the Journal contains a selection of papers from the SAIMM Pyrometallurgical Modelling conference. These papers should provide a good sample of the current activities in this very dynamic field. One of the challenges encountered in modelling pyrometallurgical processes is the chemical complexity of some of the feed materials and products. How best to represent coal has challenged modellers for years, but a systematic approach to this has now been adopted. Thermodynamic modelling has been applied to chemical reaction systems using diverse feed materials and reductants to produce a wide variety of metals, from platinum to clean steel. Techno-economic models bring in the economic aspects too. The extreme conditions in pyrometallurgical reactors have also proved challenging, involving not only very high temperatures, but jets of air at sonic velocity have been used in converting of PGM matte; and comparisons of modelling and industrial trials have been made. Fluid flow analysis has become more widespread and has been used to model the flow in tundishes and converters. A multi-physics approach, involving the interaction between concentration fields and a magneto-hydrodynamic description of an electric arc has been used to study the effect of dust particles in a furnace. Modelling of gas-solid reacting systems has been used to study the sintering of iron ore, as well as rotary kilns for direct reduction.

Pyrometallurgy superficially appears primitive and little changed from hundreds of years ago, but is one of the most challenging areas to understand and model. The simultaneous effects of very high temperatures, energy transfer, fluid dynamics, electromagnetics, phase changes, multiphase flow, free surface flow, particulate materials, and thermochemistry will provide much to interest pyrometallurgical modellers of the future. The dramatic increases in computing power make it possible to carry out different modelling approaches that earlier generations could only have dreamed about.

R.T. Jones
The South African Committee on Tunnelling (SANCOT) held its annual conference from 23 to 24 April 2015 under the theme of ‘Mechanised Underground Excavation in Mining and Civil Engineering’. The conference took place at the beautiful Zulu Kingdom, Elangeni Hotel in Durban, South Africa.

This conference was in response to the civil and mining industry being under immense pressure to deliver projects fast, efficiently, and as safely as possible. Mechanized underground excavation and support installation is proving to be an invaluable and cost-effective tool in project execution. Technology exists for the mechanized excavation of tunnels from as small as 300 mm to in excess of 18 m in order to access orebodies, build roads, railways, facilitate the installation of utilities, construct storage caverns for gas and oil, etc.

The conference was attended by various stakeholders involved with underground excavation, both locally and internationally, including the following:

- Shaft-sinking companies
- EPCM executives and management
- Civil construction companies
- Local municipalities and water authorities
- Engineering design and consulting companies
- Project management practitioners
- Technology suppliers and consumers
- University students.

Following the presentation of papers on 23 and 24 April, on 25 April delegates embarked on a technical site visit which presented them with the opportunity to walk through the tunnel underlying the Durban Harbour entrance, visit the adjoining pump station, and enjoy a one-hour cruise around the harbour.

From the point of view of the SANCOT Young Members’ Group (SANCOT-YMG) technically, the conference was a success. It was most encouraging to see this youth forum receiving a warm welcome and support from all stakeholders at the conference. As already identified, young professionals can make valuable contributions in the civil and mining industries. SANCOT has made a commitment to support and encourage the participation of young professionals in all its organizational activities. This way, the young professionals are also able to make a meaningful contribution towards their academic, professional, and technical development.

Primarily, SANCOT-YMG’s focus is to ensure that there is alliance and synergy, both with its mother bodies, which are SANCOT and SAIMM, and with other related organizations and professional bodies on various aspects that affect young professionals. This includes the execution of the mandate as adopted from the resolution taken at the International Tunnelling and Underground Space Association (ITA) General Assembly of 2014 in Iguassu, Brazil, which sets out the following aims:

- To provide a technical networking platform within the ITA for young professionals and students
- To bridge the gap between generations and to network across all experience levels in the industry
- To promote awareness of the tunnelling and underground space industry to new generations
- To provide young professionals and students with a voice in the ITA, including the Working Groups
- To look after the next generation of tunnelling professionals and to pass on the aims and ideals of the ITA.

As a representative of one of the 71 Member Nations in the ITA, SANCOT is expected to participate in all the Association’s activities. What is of particular interest in the forthcoming ITA’s international events is that, going forward, the young professional groups from each of the Member Nations will now be able to take part in the ITA’s activities. SANCOT-YMG will also be taking part, and will be represented by its current chairman, Mr. Lucky Nene, at this year’s International Tunnelling and Underground Space Association Young Members Group (ITA-YM) session of the ITA’s 41st General Assembly and Congress, taking place between 22 and 28 May 2015 in Dubrovnik, Croatia.

The upcoming annual meetings of the ITA General Assembly will be held at the following venues:

- Dubrovnik, Croatia: 22–28 May 2015, during the ITA-AITES WTC 2015 ‘Promoting Tunnelling in South East European Region’
- San Francisco, USA: 22–28 April 2016, during the ITA-AITES WTC 2016 ‘Uniting our Industry’

Young professionals in the tunnelling space, including those who would like to participate in general and offer assistance in the sustenance of this young professional forum, are invited to contact the SANCOT-YMG chairman directly on Lucky.Nene@aecom.com or via Raymond van der Berg on raymond@saimm.co.za.

L. Nene
C

an you believe that it is May 2015 already? Nine times out of ten, when people of an older generation are asked this question it results in an impromptu discussion including remarks such as ‘where has the time gone?’ or ‘time seems to go by faster as you get older’. All of which is nonsense from Einstein’s perspective. However, I do have my own answer to these questions and it is simple. When I was in my 20s it would probably take me five seconds to tie my shoelaces and run up a flight of stairs. Now it takes me five minutes to put on my slippers and haul myself up to the next floor – a hard reality but true for most! So it is that we find ourselves in May and I had planned to write an update of the SAiMM activities after the first six months – well eight months have flown by and I must keep my promise to myself and the Journal.

In many respects the mining industry has not had a good 2014/2015. The overall contraction in the industry filters through to all levels of activity, and the SAiMM is not immune to this process. We have seen quite a dramatic drop-off in attendance at conferences, and several planned events have had to be cancelled by our Technical Programme Committees. As I have written previously, curtailment in discretionary spending by mining companies is quite understandable. However, it is regrettable that it is the development of our young engineers that suffers the most in this respect, in that they are not able to have the opportunities of either writing and presenting papers or attending conferences and developing their network of industry contacts.

It is important to note that, based on wise investment decisions some years ago, the SAiMM is well positioned financially to continue operations without compromising our quality of work or various initiatives in the industry. This Council-sanctioned strategy is a cornerstone of the SAiMM’s ability to grow within southern Africa. However, we work in a dynamic environment, and a meeting has been scheduled whereby the operation and business model of the Technical Programme Committees will be reviewed to ensure that the SAiMM remains viable and competitive under the current circumstances.

On a much more positive note we have had good progress to report on the following activities:

**Mining Dialogues 360°**

The Mineral Economics Division of the SAiMM had been given a mandate to look at the economic issues that impacted on the minerals industry in South Africa. A report was prepared in this context a number of years ago and MD360° was established to engage with government, mining companies, and other stakeholders. An Advisory Committee of eminent persons has been established by Mr Mike Solomon and chaired by the SAiMM President in order to engage the above groups. The Advisory Committee’s objective is to assist in developing a set of agenda items that could be tabled at a national level to raise research funding in the same way as the Resource Nationalism initiative was funded.

**Investment Committee**

As mentioned above, the SAiMM’s investments have performed well and provide long-term stability to the organization. However, Council requested that Dr G. Smith, Sam Moolla, and I investigate, through independent financial advisors, whether or not we still have the appropriate investment strategy in terms of markets, bonds, and property. This exercise in nearly complete and will be reported at the next Council meeting.

**Regional Development Manager**

Some of you may not be aware that the SAiMM has employed a Regional Development Manager in a part-time position. Over several years now we have been working on establishing sustainable branches in Zambia, Zimbabwe, Namibia, Botswana, and the DRC. Considerable effort has been expended on this by the Johannesburg office as well as our Officers and Members in these countries. In order to meet the increasing demands of supporting these new organizations and to ensure that the marketing of the SAiMM is managed evenly across the region, Council approved the employment of a dedicated and knowledgeable person. Malcolm Walker has filled this role since October 2014 and has actively supported the SAiMM office. He has specifically focused on reaching out to all of the appropriate universities in the region and we have had an excellent response.

**SAMREC and SAMVAL COMMITTEE (SSC)**

The SSC has been fulfilling an important role for the Johannesburg Stock Exchange for several years. Over this time the structure has developed and matured, and the Geological Society of South Africa and the SAiMM have met during the year to determine what (if anything) needs to be done to further support the initiative. This resulted in the establishment of an appropriate budget and an updated Terms of Reference for the SSC. The final drafts of these documents will be tabled at the SSC meeting on 28 May 2015.

One of the structures that is required by both the by-laws of the SAiMM and the ToR of the SSC is an effective process for the handling of complaints about professional conduct. This had not received the appropriate attention of the SAiMM in the past, and a duly elected and appointed Complaints Committee and Ethics Committee will be approved at the next Council meeting.

There are many other items to comment on relating to the Young Professionals Committee, our relationship with ECSA, etc., but I fear I am running out of space and … time. I only type slowly!

J.L. Porter
President, SAiMM
Jos Lurie, an honorary life Fellow of the Southern African Institute of Mining and Metallurgy passed away on Monday 27 April 2015 at the age of 86 after his fight with cancer.

From his early childhood in Maclear in East Griqualand Jos challenged the world and showed his leadership qualities in the Scouts and through independent camping adventures. His youthful experiences are recorded in an unpublished book he wrote in the last full year of his life, entitled ‘An Exciting Life’, which I was privileged to proofread. This was typical of Jos recording all his activities and contributions made during his ‘exciting life’.

His first employment was as a filing clerk, followed by a job as a trainee draftsman – he qualified in 1947. He progressed through his own efforts to the Department of Trigonometrical Survey in Mowbray, Cape Town, where he extended his skills to surveying and obtained distinction in the survey course, including photogrammetry. While in Cape Town his adventurous spirit prevailed, with weekly climbs of Table Mountain.

His survey excellence was built up in Zululand and the Cape and culminated in his obtaining employment in 1954 as an engineering surveyor in Kenya to set up irrigation schemes. During this 4-year period Jos learned to fly small planes and had the opportunity to climb the Kilimanjaro parasite volcanic peak of Kibo (5890 m), the highest altitude in Africa, in ‘record time’, accompanied by only one other friend. He was always an adventurer!

Jos met and married Brenda, his wife of 57 years, in 1958. Brenda was an English nursing sister from Surrey, who was in the middle of a nursing contract in Kenya at that time. Their honeymoon took them on an adventure in a Land Rover through Central Africa during turbulent political times before they decided to return to SA. In Grahamstown, Jos studied geology while being supported by Brenda, and graduated BSc (Hons) with distinction in 1961.

In 1963 Jos chose the option of education as a future career and joined the staff of the Witwatersrand Technical College as lecturer in geology and surveying. This has been his life and enthusiasm ever since.

Jos was passionate about vocationally based technical engineering education in particular. He was a competent practical and theoretical geologist, gemmologist, and surveyor of the highest order. He was the Head of the School of Mines from 1980 for more than 20 years, after which in semi-retirement he continued active engagement up until 2014. He was a highly respected academic, a prolific author, and researcher whose works will no doubt continue to influence the world. He was well travelled and shared most of his travels with Brenda by his side.

Jos was an honorary Life Fellow of the SAIMM, which recognized his service to the Institute from 1980 to his ‘first retirement’ in 1990. He never gave up his interest in education, with courses being offered up until late 2014 when he first became ill.

During his tenure at Technikon Witwatersrand he carried out a specialist study on the Pilanesberg on rare earth deposits, culminating in a PhD award in 1974. Again, the support of Brenda was always recognized by Jos. He remained an acknowledged expert in this field throughout his life, and has left comprehensive materials to support future possible mining ventures.

Such activities not being enough to satisfy Jos, he set to writing technical books for publication, which included:

- History of Mining and Metallurgy at Technikon Witwatersrand (1980)
- SA Geology for Mining, Metallurgical and Hydrological and Civil Engineering (1977) (11 editions)
- Technikon Witwatersrand – A History 1925–2000
- Symetrix Dynamic 3D Model Maker (2012)
- Symmetrical Polyhedra (2008)

He had more than 15 published technical papers and reports as well as many conference presentations across the world, ranging from hydrology in Kenya to microscopic mineral analysis, a new football (just prior to the SA World Cup activities in 2010), and synthetic gems.

The record (unpublished) of his ‘Exciting Life’ will be a tribute to him and is a fitting end to not only an exciting life, but a life of contribution and success and an inspiration to those that follow him.

He is survived by his wife Brenda and their son Ross and daughter Wendy.

P. Knottenbelt
Industry and Government support for Electra Mining Botswana

Leading local and international suppliers to the industrial and mining sectors will gain valuable exposure to the southern African mining market at Electra Mining Botswana 2015. Exhibitors at the show will have the opportunity to network with key decision-makers from Botswana’s growing industrial and mining sectors, position their company brand, grow their client base, and launch new products and services directly to their target market.

Botswana’s thriving mining and industrial sectors makes it the natural choice for companies such as Joy Global (Africa), Verder Pumps, Filtration Africa, Air Liquide Botswana, Franklin Electric, Becker Mining South Africa, Jachris Hose and Couplings, Schnieder Electric South Africa, Charnaud, Tubestone, and AC/DC Dynamics, among many others, to exhibit at Electra Mining Botswana.

In addition to leading companies participating at the show, the Government of Botswana is also backing the event.

‘We’re proud to announce that the Botswana Ministry of Minerals, Energy and Water Resources has confirmed its endorsement of Electra Mining Botswana,’ says Gary Corin, Managing Director of Specialised Exhibitions Montgomery, organizers of the show. ‘The Ministry has expressed the importance of the exhibition to the mining, construction, and power generation industry because it brings major technology partners and suppliers together.’

Onthusitse H. Melaetsa, Permanent Secretary at the Ministry of Minerals, Energy and Water, says that ‘the event will assist the mining industry to strengthen relationships, source and view the latest technologies available to the sector as well as source project finance and funding.’

‘This event fills a vacuum that existed in Botswana,’ says Mmetla Masire, Coordinator Relocation & Opportunities at the Ministry of Minerals, Energy and Water. ‘It now brings a show that is dedicated and specialized in the mining, power generation, and related industries and I would highly recommend it to potential exhibitors and those wanting to see the latest offerings in the market.’

Also endorsing Electra Mining Botswana is Botswana Chamber of Mines CEO Charles Siwawa, who says that ‘the objective of the show is to assist the mining industry in strengthening stakeholder relationships. In addition to the exhibits there will be interesting seminars taking place concurrently during the three-day exhibition.’

The exhibitor profile will include mining and related products, industrial engineering and manufacturing, general engineering and manufacturing, electrical engineering and power generation, materials handling, safety, health, and environment, and construction. The show will also feature exciting free-to-attend seminars that will provide a wealth of information and interactive discussion.

‘The exhibition embraces mining, industrial, power generation, and construction and will play a vital role in growing Botswana’s already thriving mining and industrial economy, bringing related industries together at one location for visitor and exhibitor convenience,’ concludes Corin.

Taking place from 1–3 September at the Gaborone Fair Grounds in Gaborone, the power hub of Botswana, the exhibition is organized through a joint venture between Soapbox Communications, a local Botswana company, and Specialised Exhibitions Montgomery, a South African company with over 42 years of exhibition experience.

For more information, contact Charlene Hefer, Portfolio Director: Mining and Industrial, Specialised Exhibitions Montgomery, at email charleneh@specialised.com

C. Tointon
RHI is the leading global partner for the nonferrous metal industry. We offer the complete programme of most exclusive products and service ranges from basic and non basic bricks, carbon blocks, as well as non shaped products, prefabricated products, slide gate plates and purging plugs.

Our clients can rely on our state-of-the-art all inclusive solutions for processes, lining concepts, special machinery equipment and repair systems as well as computer simulations like CFD, FEA and thermodynamic calculations to support the improvement of metallurgical processes and furnace integrity.
Pyrometallurgy Papers

Representation of coal and coal derivatives in process modelling
by J.A. Theron and E. le Roux ................................................................. 339

This paper provides guidelines on mass and energy balance modelling involving coal and coal derivatives. Several potential pitfalls of such modelling processes are outlined. It is recommended that an ‘enthalpy correction value’ is incorporated in energy balances involving combustion, devolatilization, or conversion of coal and coal derivatives.

Sonic injection into a PGM Peirce-Smith converter; CFD modelling and industrial trials

Western Platinum conducted a numerical assessment, followed by a full-scale industrial evaluation, of implementing sonic injection into a Peirce-Smith converter as part of its operational improvement and energy reduction initiatives. The paper discusses the key findings in understanding plume extension, velocity distribution, shear wall stress analysis, and phase distribution characteristics in the system.

Physical and numerical modelling of a four-strand steelmaking tundish using flow analysis of different configurations
by J.H. Cloete, G. Akdogan, S.M. Bradshaw, and D.K. Chibwe ................................................................. 355

The flow behaviour in a four-strand tundish was investigated using a ½-scale water model as well as numerical modelling. The numerical and physical model were used to characterize the residence time distribution and calculate the properties pertaining to the tundish flow under three different tundish configurations.

Modelling of fluid flow phenomena in Peirce-Smith copper converters and analysis of combined blowing concept
by D.K. Chibwe, G. Akdogan, P. Taskinen, and J.J. Eksteen ................................................................. 363

This investigation consists of a numerical and physical modelling exercise on flow patterns, mixing, solid-liquid mass transfer, and slag-matte phase distribution in a 0.2-scale cold model of an industrial Peirce-Smith converter. Mass transfer measurements indicated that the fluid flow in the converter is stratified. Blowing configuration and slag volume have significant effects on mixing propagation, wave formation, and splashing. A combined blowing configuration using top-lance and lateral nozzles is proposed to increase process efficiency.

The recovery of platinum group metals from low-grade concentrates to an iron alloy using silicon carbide as reductant
by W. Malan, G. Akdogan, S. Bradshaw, and G.A. Bezuidenhout ................................................................. 375

Base metals and PGMs can be recovered in an iron alloy by silicon carbide reduction of a low-grade platinum concentrate with converter slag additions. Integrating such a process into the matte-based collection process could be considered as an alternative in the future smelting of low-grade UG2 concentrates.

Value-in-use model for chlorination of titania feedstocks
by S. Maharajh, J. Muller, and J.H. Zietsman ................................................................. 385

A techno-economic model was developed to describe the chlorination process for TiO2 pigment production and estimate the process variables at steady state. The model can be used to quantify the effects of using different feedstocks.

Interaction of dust with the DC plasma arc – a computational modelling investigation
by Q.G. Reynolds ................................................................. 395

A continuum model was developed for dust transport in the arc region of DC plasma arc furnaces. Qualitative case studies produced a number of practical suggestions for furnace operation, including increased dust capture by the bath when feed ports are located closer to the electrode, and the possible effects of feed segregation in the furnace freeboard based on dust particle size and density.

A finite difference model of the iron ore sinter process
by J. Muller, T.L. de Vries, B.A. Dippenaar, and J.C. Vreugdenburg ................................................................. 409

A model of the iron ore sintering process has been developed that uses the finite difference method (FDM) to evaluate the behaviour of specific iron ore sinter feed mixtures. The model aims to predict sinter quality, including chemical quality and physical strength, as well as key sinter process performance parameters such as production and fuel consumption rates.

Modelling and optimization of a rotary kiln direct reduction process
by H.P. Kritzinger and T.C. Kingsley ................................................................. 419

This paper illustrates the application of numerical optimization techniques in combination with a rotary kiln model in the interrogation of a generic iron-ore reduction process. The fundamental modelling concepts are explained, followed by a description of the optimization approach.

These papers will be available on the SAIMM website
http://www.saimm.co.za
General Papers

Equipment selection based on the AHP and Yager’s method
by M. Yavuz .......................................................... 425

Loader equipment for the Aegean Lignite Colliery was selected by using both the analytic hierarchy process and Yager’s method. A sensitivity analysis was applied for each method in order to see how the selection criteria affect the final decision. The advantages and disadvantages encountered during the application of each decision-making process are presented.

Pre-sink shaft safety analysis using wireline geophysics
by N. Andersen .......................................................... 435

This paper outlines how rock mass characteristics, in-situ rock stress, rock strength, hydrological characteristics, and structural parameters can be determined using wireline logging of a vertical, pre-sink diamond drill-hole. The ‘stick plot’ method is introduced as a reporting method that combines all geotechnical parameters applicable to the stability of the proposed shaft into an easily readable format.

Hydraulic support instability mechanism and its control in a fully-mechanized steep coal seam working face with large mining height
by Y. Yuan, S.H. Tu, F.T. Wang, X.G. Zhang, and B. Li .......................................................... 441

This paper focuses on the analysis of hydraulic support instability (HSI) types, the key parameters and techniques to control HSI in fully-mechanized mining faces with large mining height, the establishment of a model of HSI, and a multi-parameter sensitivity mechanical model of different HSI types on a longwall coal mining face.

Unplanned dilution and ore loss prediction in longhole stoping mines via multiple regression and artificial neural network analyses
by H. Jang, E. Topal, and Y. Kawamura .......................................................... 449

Models for the prediction of unplanned dilution and ore loss are established using multiple linear and nonlinear regression analyses, as well as an artificial neural network (ANN) method. It is shown that the proposed ANN model can be directly used as a practical tool to predict unplanned dilution and ore loss, which will not only enhance productivity, but also be beneficial for stope planning and design.

Numerical simulation of multiphase flow in a Vanyukov furnace
by H.L. Zhang, C.Q. Zhou, W.U. Bing, and Y.M. Chen .......................................................... 457

A multiphase model of the flow in a Vanyukov furnace was built using computational fluid dynamics (CFD) software and solved with the volume of fluid (VOF) and $k - \varepsilon$ model. The proposed model can be used to predict the multi-phase movement, slag/air fluctuation, vortex formation, and the effects of changes to the structural and operational parameters, and provides a method for optimization of the furnace structure and operating conditions.
Representation of coal and coal derivatives in process modelling

by J.A. Theron* and E. le Roux*

Synopsis
This paper provides guidelines on performing mass and energy balance modelling involving coal and coal derivatives. Usually, the inputs to a pyrometallurgical process would be specified in terms of elements and compounds. Reliable thermochemical data is more widely available for species involving uniquely defined, relatively smaller molecules. However, in the case of coal, the molecules are extremely large and not uniquely defined. Consequently, modelling processes involving coal and its derivatives involve several potential pitfalls. These are outlined in the present paper.

It was found that coal proximate analysis should not be regarded as absolute; it could vary with several parameters, including heating rate. For modelling, the use of ultimate analyses should be considered a preferable option to proximate analyses, where ‘fixed carbon’ and ‘volatiles’ are not defined in terms of chemical composition. Significant errors could be incurred if the larger molecules are neglected during calculation of the calorific value (CV) of coal gas (the gas liberated when coal is heated in the absence of oxygen).

For elemental analysis determination, the oxygen content (which is calculated by balance) should be checked to ensure it is within the expected range. For representation of sulphur in coal, one should avoid double-counting due to SO$_2$ in the ash analysis.

Potentially, oxygen in coal could be represented as O$_2$, H$_2$O, CO, or CO$_2$. However, use of some of these species without considering the experimentally determined gross CV leads to significant errors in the energy balance. If coal enthalpy is calculated from elemental analyses without correction, representation of coal oxygen as H$_2$O(l) gives reasonable accuracy. Coal volatiles could be represented by a complex mixture of compounds, even using different oxygen-containing species than these four, provided the enthalpy is corrected.

It is recommended that an ‘enthalpy correction value’ be incorporated in energy balances involving combustion, devolatilization, or conversion of coal and coal derivatives, e.g. coke, char, tar, or tar. That would imply that proximate analysis, elemental analysis, as well as the gross CV would be provided the enthalpy is corrected.

Keywords
cell properties, process modelling, proximate analysis, energy balance, enthalpy.

Introduction
Coal is possibly the most heterogeneous substance used in the minerals industry, especially that sector involving processing at high temperatures. Coal derivatives include coke, char, tar, pitch, and coal gas which are important commodities in industry.

Coal is used extensively in the metallurgical industry for widely different purposes, e.g. electrical power generation, reductant manufacturing (coke and char), as well as gasification, which allows the value of coal to be extended to a wide range of chemical products. Pulverized coal injected into the blast furnace (for the purpose of decreasing coke consumption) is subjected to significantly different conditions than pulverized coal used for power generation. Reductants such as anthracite fed to an open arc smelting process are subjected to rapid rates of heating. Lump coal fed into the Corex (Institute for Industrial Productivity, 2012a), smelt-reduction, or rotary kiln direct reduction (DR) processes (Institute for Industrial Productivity, 2012b) is subjected to reducing conditions as well as a relatively rapid rate of heating.

It is therefore important to understand the physiochemical properties of coal as they relate to different applications in order to extract maximum value from available coal resources. Process modelling plays an important role in extracting this value through a detailed understanding of the quality and physiochemical properties of coal and its derivatives. This paper highlights some of the relevant issues and potential pitfalls in the modelling of coal, focusing on the application of proximate and ultimate analysis of coal, with specific reference to oxygen content, and the effect of different assumptions regarding its representation on the calculated calorific value (CV).

Current evaluation methods for coal include proximate analysis, total sulphur, and CV. Proximate analysis includes moisture, volatiles, ash, and fixed carbon yields. (Note the preference for the word ‘yields’ in this context, as opposed to ‘contents’. That is because coal actually contains minerals and not ash. Ash is the remnants of minerals after...
complete oxidation of the coal. Most often these analyses are not adequate to fully describe the behaviour of the coal in the specific process. Technologists, especially in the fields of power generation and coke-making, properly consider the results of a number of additional tests, e.g. elemental analyses, ash analysis, ash fusion temperature, and coal petrography. Coke-makers consider coal plasticity tests (e.g. Gieseler fluidity and dilatation), and those involved in power generation consider coal reactivity, especially from drop tube oven results.

The use of mathematical modelling in metallurgical and chemical processes

Mass balance modelling is simply based on the law of conservation of mass. Although the concept is simple, there are potential pitfalls associated with these calculations, especially for coal. The same applies to energy balances, which are based on the enthalpy function. Considerable time has elapsed since the initial development of the field of thermodynamics and introduction of, for example, the concept of Gibbs free energy (Bodner Group, 2014). Nowadays, exploiting the concept of Gibbs free energy minimization is easier than previously, due to the availability of useful databases, software, and computers.

Usually one would specify an input to a pyrometallurgical process in terms of elements and compounds. However, in the case of coal the molecules are extremely large, and not uniquely defined. Reliable thermochemical data is more widely available for species involving uniquely defined, relatively simpler molecules.

Nevertheless, it is essential to understand the limitations of mathematical modelling. The quality of the output depends on the following:

- Accuracy of inputs
- Understanding of the process
- Validity of assumptions
- Intent of the model
- Inherent limitations of modelling
- The level of skill of the person undertaking the task, including the use of checks and balances
- The time allowed for execution of the task, which if not enough, could force the person to make unjustified assumptions.

Proximate analysis

Moisture content

Preparation of a new coal sample would include air-drying the coal at ambient temperatures or at elevated temperatures not exceeding 40°C (SANS 589:2009, 2009). The apparently dry coal obtained is referred to as ‘air-dry’. The mass loss from wet coal to ‘air-dry’ coal is referred to as ‘free moisture content’. A sample of air-dry coal, after appropriate sample preparation techniques (including milling), is heated to a temperature of between 105ºC and 110ºC, and the associated mass loss is referred to as ‘residual or inherent moisture’. The sample is then referred to as ‘dry’ or ‘absolutely dry’. Total moisture content of the coal sample is calculated as follows:

\[
\text{%Total moisture} = \text{%Free moisture} + \text{%Inherent moisture} \quad [1]
\]

Some coals liberate additional moisture (water of crystallization) when heated to temperatures higher than about 105°C. This moisture reports as part of the volatile content. In the case of highly porous coal derivatives such as coke or char, the drying method prescribes temperatures between 120°C and 200°C, with additional care to ensure that no further mass loss occurs before recording the mass (SANS 579:2005, 2005).

Proximate analysis calculation

Proximate analysis is usually carried out on an air-dry coal sample. Results include inherent moisture, volatiles, and ash yields, while the balance is allocated to fixed carbon, with all values expressed on an air-dry basis, as follows (SANS 17246:2011, 2011):

\[
\%\text{Fixed C} = 100\% - (\%\text{Moisture} + \%\text{Volatiles} + \%\text{Ash}) \quad [2]
\]

Note that sulphur remaining in the residue would report to ‘fixed carbon’. The values on an air-dry basis could be converted to an absolute dry base, e.g. by applying the following conversion:

\[
\%\text{Fixed C}_{\text{dry}} = \frac{\%\text{Fixed C}_{\text{air dry}}}{1 - (\% \text{Inherent moisture})/100} \quad [3]
\]

During modelling and reporting of modelled results, care should be exercised to specify all analyses as ‘wet as-received’, ‘air-dry’, or ‘dry’ and to use the appropriate conversion factors to avoid errors.

Coal volatiles

During determination of the volatile content of coal, a small milled sample is inserted in a crucible and covered by a lid. The crucible is loaded into a muffle furnace at 900°C for a duration of 7 minutes (SANS 50:2011, 2011). The mass lost, after subtracting the moisture content, is referred to as ‘volatiles content’ or volatiles yield.

For determination of ash yield, the coal is subjected to oxidizing conditions. The temperature is limited to 850°C to minimize the loss of volatile compounds such as K2O and Na2O.

According to Rosenqvist (1974), ‘The proximate analysis gives the percentage of “moisture”, “volatile matter”, “fixed carbon” and “ash”. Each of these is determined by standardized procedures, and different values would be obtained if different procedures were used.’ Procedures were standardized by ISO, ASTM, and other organizations.

Some operators who are less familiar with coal could treat the results from proximate analyses as if they were absolute. However, considering the quote from Rosenqvist and observing the extent to which actual processes differ from the procedures for proximate analysis, behaviour not in line with proximate analysis should actually be expected. Therefore it should not be surprising if the actual performance of coal, e.g. during charring or coke-making, deviates from what would be expected if the characteristic were calculated on the basis of the proximate analysis.

One example of actual results deviating from proximate analysis data is the observation that rapid heating tends to increase the volatile yield. Most noticeably, that decreases the yield of fixed carbon (Niksa, 1995).

Composition and representation of volatiles

Coal volatiles are partly organic and partly inorganic in origin. Water vapour and carbon dioxide from clay and carbonate
minerals are the main inorganic volatiles. Some effects of inorganic volatiles are as follows:

- They do not contribute combustible species that could increase the CV.
- Their liberation could be associated with endothermic reactions, which would neutralize part of the exothermic reaction heat from combustion.
- They could adversely affect ignition of the coal.

Not all the water from clays is liberated at approximately 105°C, as the remainder (crystal water) is bound in chemical compounds that decompose at higher temperatures. These volatiles of inorganic origin are referred to as ‘inert volatiles’ (Porter and Ovitz, 2014). Coal volatiles could also be subjected to secondary reactions after initial liberation – for example, in the case of tar from slot coke-making ovens, in which thermal cracking occurred during contact with surfaces at a higher temperature than that of initial release. Thermal cracking (Chiu and Hong, 1983) involves the formation of pyrolytic carbon, smaller molecules (such as H2), and modified hydrocarbon compounds. Pyrolytic carbon is deposited in the coke pores during carbonization, which increases the yield of fixed carbon significantly (Chiu and Hong, 1983). If the process being modelled involves thermal cracking, appropriate assumptions would be required, which should be based on evidence from experimental work or plant observations.

Condensable hydrocarbons in coal volatiles represent a modelling challenge. Condensable hydrocarbons contain numerous compounds, for which detailed analyses are seldom available. Tars in particular contain numerous compounds with very large molecular structures and which are thermally unstable. Representation of tar with a simpler species or mixture of species of smaller molecular mass with well-known thermodynamic data is advantageous. In this regard it could be mentioned that benzene (C6H6) has a high carbon content of 92.3%, in the same order of magnitude than typical tar from slot coke-making ovens. For quick calculations where approximate results are required, benzene could be used to represent tar. Light oils, also referred to as BTX, contain benzene, toluene, and xylene. As benzene predominates in the composition of these light oils, it could also represent this group of compounds where approximate results are required (Powell, 1945).

### Representation of volatiles for coal gas CV calculation

The large molecules of condensable hydrocarbons do not make a major contribution to the volume of coal gas. However, they do make a significant contribution to both the CV and carbon content of the gas. According to Powell, typical coke oven gas from a by-product coke oven contains about 0.65% by volume light oils (after tar removal, but before BTX removal) (Powell, 1945).

In Table I, composition by volume of coal gas from a typical by-products coke-making oven, given by Powell, is presented, together with the percentage contribution of each individual component of that gas analysis to the calculated CV of the gas mixture (23.95 MJ/Nm³ in this instance). If only the contributions of hydrogen, carbon monoxide, and methane are taken into account, the calculated gas CV would be only 82.5% of the accurate value, assuming that the given calculated value is the accurate one. Light oils, which represent only 0.65% of the volume of the gas, contribute almost 4% of the gas CV.

Similarly, in Table II, composition by volume of coal gas from low-temperature carbonization (Powell, 1945) is presented. This gas has an even higher CV of 27.5 MJ/Nm³, compared to 23.9 MJ/Nm³ for by-product coke oven gas. Similar to the case of low-temperature carbonization, hydrogen, carbon monoxide, and methane contribute only 67.8% of the gross CV. The contributions, especially by substances containing at least two carbon atoms, are large and omission of them would result in significant errors. In the case of low-temperature carbonization gas, light oils represent about 1.5% of the gas volume; however, they contribute almost 8% of the gas CV.

### Table I

<table>
<thead>
<tr>
<th>Species in unwashed coke oven gas from by-products plant</th>
<th>Volume % of gas species</th>
<th>% Contribution to gross CV</th>
<th>% Combined contribution to gross CV</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hydrogen H2</td>
<td>56.70</td>
<td>30.24</td>
<td>82.5</td>
</tr>
<tr>
<td>Methane CH4</td>
<td>29.60</td>
<td>49.17</td>
<td></td>
</tr>
<tr>
<td>Nitrogen N2</td>
<td>0.90</td>
<td>0.00</td>
<td></td>
</tr>
<tr>
<td>Carbon monoxide CO</td>
<td>5.70</td>
<td>3.05</td>
<td></td>
</tr>
<tr>
<td>Carbon dioxide CO2</td>
<td>1.70</td>
<td>0.00</td>
<td></td>
</tr>
<tr>
<td>Ethylene C2H4</td>
<td>2.45</td>
<td>6.45</td>
<td></td>
</tr>
</tbody>
</table>

### Table II

<table>
<thead>
<tr>
<th>Gas species</th>
<th>Volume % of gas species</th>
<th>% Contribution to gross CV</th>
<th>% Combined contribution to gross CV</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ethane C2H6</td>
<td>1.28</td>
<td>3.72</td>
<td>13.59</td>
</tr>
<tr>
<td>Propane C3H8</td>
<td>0.34</td>
<td>1.31</td>
<td></td>
</tr>
<tr>
<td>Butane C4H10</td>
<td>0.02</td>
<td>0.11</td>
<td></td>
</tr>
<tr>
<td>Acetylene C2H2</td>
<td>0.05</td>
<td>0.12</td>
<td></td>
</tr>
<tr>
<td>Hydrogen sulphide H2S</td>
<td>0.70</td>
<td>0.73</td>
<td></td>
</tr>
<tr>
<td>Oxygen O2</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>Light oils C6H6*</td>
<td>0.65</td>
<td>3.96</td>
<td>3.96</td>
</tr>
</tbody>
</table>

* Benzine represents light oils.

**Table I**

<table>
<thead>
<tr>
<th>Coal gas composition from by-product coke oven and its contribution to gross calorific value (Powell, 1945)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Species in unwashed coke oven gas from by-products plant</td>
</tr>
<tr>
<td>--------------------------------------------------------</td>
</tr>
<tr>
<td>Hydrogen H2</td>
</tr>
<tr>
<td>Methane CH4</td>
</tr>
<tr>
<td>Nitrogen N2</td>
</tr>
<tr>
<td>Carbon monoxide CO</td>
</tr>
<tr>
<td>Carbon dioxide CO2</td>
</tr>
<tr>
<td>Ethylene C2H4</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Minor and trace gas constituents</th>
<th>Volume % of gas species</th>
<th>% Contribution to gross CV</th>
<th>% Combined contribution to gross CV</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ethane C2H6</td>
<td>1.28</td>
<td>3.72</td>
<td>13.59</td>
</tr>
<tr>
<td>Propane C3H8</td>
<td>0.34</td>
<td>1.31</td>
<td></td>
</tr>
<tr>
<td>Butane C4H10</td>
<td>0.02</td>
<td>0.11</td>
<td></td>
</tr>
<tr>
<td>Acetylene C2H2</td>
<td>0.05</td>
<td>0.12</td>
<td></td>
</tr>
<tr>
<td>Hydrogen sulphide H2S</td>
<td>0.70</td>
<td>0.73</td>
<td></td>
</tr>
<tr>
<td>Oxygen O2</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>Light oils C6H6*</td>
<td>0.65</td>
<td>3.96</td>
<td>3.96</td>
</tr>
</tbody>
</table>

Gas CV including all components: 23.93 MJ/Nm³
Representation of coal and coal derivatives in process modelling

Liberation of volatiles at high temperatures

The residue from the proximate analysis test in which ‘volatiles’ were determined is by no means free from volatile elements like H, O, N, and S. Most of the remaining volatile elements are liberated only at temperatures higher than 900ºC, and even exceeding 2000ºC. In a Lurgi packed-bed gasifier sampling campaign, Bunt and Waanders found that 10% of the coal nitrogen, as well as 0.75% of coal hydrogen, remained in the residue after reaching a temperature of at least 1000ºC (Bunt and Waanders, 2008).

For a detailed mass balance on a process that produces reductants, or even one where coal is converted to char for consumption in the process itself, such as the DR kiln, the extent of liberation of H, O, N, and S, as well as the remaining carbon that is associated with the volatiles, should be carefully considered.

If coke or char is heated to very high temperatures (higher than e.g. 1500ºC) in the absence of oxygen to effect graphitization or to drive off the remaining H, N, S, and O, the ash composition could also be expected to change. Volatile oxides (such as K$_2$O and Na$_2$O) would be driven off to a large extent. Most remaining ash oxides could react with carbon at these temperatures, forming volatile oxides such as SiO(g) and Al$_2$O(g). A notable exception to this behaviour is iron, which does not readily form a volatile reaction product. Under such conditions, iron would exist in the reductant as metallic iron or perhaps FeS (instead of an oxide of iron). That explains why the ash composition of graphite has a significant or dominant Fe$_2$O$_3$ content (during determination of the ash composition, iron or FeS would oxidize to form Fe$_2$O$_3$). Another effect of these high-temperature reactions is the consumption of some carbon in forming these volatile oxides.

Ultimate (elemental) analysis

The char residue from the proximate analysis test for determination of ‘volatiles’ is by no means free from volatile elements like H, O, and N. Therefore ‘fixed carbon’ is not defined in terms of its elemental composition. As we have seen, ‘volatiles’ is also not defined in terms of elemental composition.

For mass and energy balance studies it is advisable to base calculations on the ultimate analysis instead of the proximate analysis of the coal. Reasons for this include the following:

➤ The percentage fixed carbon could be a function of certain parameters such as heating rate, gas pressure, and secondary reactions involving the volatiles
➤ The composition of ‘fixed carbon’ is not defined in an elemental sense, as it could contain residual sulphur, hydrogen, nitrogen, and oxygen
➤ The composition of ‘volatile matter’ is also not defined in an elemental sense, as it could contain numerous compounds in varying quantities.

Ultimate analysis involves determination of the carbon, hydrogen, nitrogen, and total sulphur content of air-dry coal. Ash (from the proximate analysis) is also used in the formula. Oxygen is determined as the balance of the elemental analysis, as follows:

%O = 100% - % Inherent moisture - %Ash - %C - %H - %N - %S

[4]

Note that neither oxygen nor hydrogen contained in the inherent moisture, nor in the ash-forming oxides, form part of the reported coal oxygen content (ASTM Designation D 3, n.d.).

For elemental analysis done on a Leco apparatus, it is important to ensure the apparatus is calibrated with a sample.

---

**Table II**

<table>
<thead>
<tr>
<th>Species</th>
<th>Volume % of gas species</th>
<th>% Contribution to gross CV</th>
<th>% Combined contribution to gross CV</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hydrogen</td>
<td>H$_2$</td>
<td>33.5</td>
<td>15.5</td>
</tr>
<tr>
<td>Methane</td>
<td>CH$_4$</td>
<td>32.0</td>
<td>46.8</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>N$_2$</td>
<td>1.1</td>
<td>0.0</td>
</tr>
<tr>
<td>Carbon monoxide</td>
<td>CO</td>
<td>11.7</td>
<td>5.4</td>
</tr>
<tr>
<td>Carbon dioxide</td>
<td>CO$_2$</td>
<td>11.0</td>
<td>0.0</td>
</tr>
<tr>
<td>Ethylene</td>
<td>C$_2$H$_4$</td>
<td>0.92</td>
<td>2.11</td>
</tr>
<tr>
<td>Ethane</td>
<td>C$_2$H$_6$</td>
<td>3.80</td>
<td>9.61</td>
</tr>
<tr>
<td>Dimethylethylene (2 isomers)</td>
<td>C$_3$H$_6$</td>
<td>0.51</td>
<td>2.25</td>
</tr>
<tr>
<td>Propylene</td>
<td>C$_3$H$_6$</td>
<td>0.87</td>
<td>2.90</td>
</tr>
<tr>
<td>Propane</td>
<td>C$_3$H$_8$</td>
<td>1.33</td>
<td>4.79</td>
</tr>
<tr>
<td>Butane</td>
<td>C$_4$H$_10$</td>
<td>0.28</td>
<td>1.31</td>
</tr>
<tr>
<td>Isobutane</td>
<td>C$_4$H$_10$</td>
<td>0.09</td>
<td>0.42</td>
</tr>
<tr>
<td>1,3-Butadiene</td>
<td>C$_6$H$_8$</td>
<td>0.02</td>
<td>0.01</td>
</tr>
<tr>
<td>Acetylene</td>
<td>C$_2$H$_2$</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>Hydrogen sulphide</td>
<td>H$_2$S</td>
<td>1.00</td>
<td>0.91</td>
</tr>
<tr>
<td>Oxygen</td>
<td>O$_2$</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>Light oils</td>
<td>C$<em>6$H$</em>{14}$</td>
<td>1.48</td>
<td>7.94</td>
</tr>
<tr>
<td>Total percentage</td>
<td>100.33</td>
<td>100.00</td>
<td>100.00</td>
</tr>
</tbody>
</table>

Gas CV including all components: 27.53 MJ/Nm$^3$

*: Benzine represents light oils.
that more or less resembles the sample being tested. If, for example, an anthracite sample is analysed while a bituminous coal reference sample is used, significant error could occur. Such an error is often evident from the oxygen content (which is calculated by difference), which can sometimes be reported as a negative value. Figure 1 shows typical oxygen contents of South African coals plus four imported hard coking coals (Schoeman and Boshoff, 1996), and Table III contains the proximate and ultimate analyses, as well as the calorific values, of this set of data. The lowest oxygen contents were found for anthracites, ranging from zero to 2%. Note, however, that oxygen contents up to about 4% are not uncommon for anthracitic coals. Hard coking coals generally have relatively high rank and high vitrinite content (Falcon, 2013) and low oxygen contents, of the order of 2–4%.

Other South African bituminous coals have oxygen contents of generally between 7% and 11%. High-inertinite coals from the Free State have relatively high oxygen contents of about 9%, and are also noteworthy due to high ash (a relatively high ash content implies a relatively low carbonaceous content).

If the ultimate analysis is used to represent coal or coal derivatives entering a process, additional care would have to be taken, especially regarding sulphur and oxygen.

**Representation of sulphur in coal**

As mentioned previously, 'fixed carbon' would also include sulphur reporting in the residue of the proximate analysis test. Under the oxidizing conditions in a pulverized fuel boiler, sulphur could be oxidized to SO2, which generally involves exothermic reactions. However, under the reducing conditions prevailing in the blast furnace or Corex processes, sulphur cannot be oxidized to SO2, but forms H2S instead. Consequently, oxidation of that part of the 'fixed carbon' cannot contribute to any exothermic heat generated for those processes. Sulphur in coal can exist in pyritic, sulphatic, and organic forms. Under oxidizing conditions, organic and pyritic sulphur would oxidize exothermally to SO2. However, sulphatic sulphur is already in an oxidized form. Sulphatic sulphur does not constitute a high percentage of the sulphur in South African coals (Schoeman and Boshoff, 1996).

It is advisable to use the total sulphur content from the elemental analysis as input sulphur into a model. Using the SO3 from the ash analysis could imply that part of the sulphur would be double-counted. On the other hand, omitting SO3 would cause missing mass in the mass balance, which is probably preferable to double-counting sulphur. SO3 in the ash is particularly related to calcium, which combines sulphur as CaSO4. Calcium sulphate forms during the ashing of the coal for ash composition determination; however, it would not necessarily form in any given process. Generally, CaSO4 would form at temperatures of around 900°C under oxidizing conditions.

If coal is devolatilized instead of combusted, reducing conditions prevail and pyrite would decompose at temperatures in the range 500–600°C (Rausch, 1975) according to:

\[
\text{FeS}_2 \rightarrow \text{FeS} + \frac{1}{2} \text{S}_2(g) \quad [5]
\]

This would affect the analysis of forms of sulphur, a topic that is beyond the scope of this paper.

Presumably, basing a representation of coal on the mineralogical analysis would be the ultimate goal. The percentage of mineral matter in the coal could be linked by approximation with the ash, as well as certain other parameters, by the King-Maries-Crossley formula (Karr, 1978), provided those parameters are available:

\[
\text{MM} = 1.09 A + 0.52 P + 0.84 \text{CO}_2 - 1.1 \text{SO}_3 + 0.5 \text{Cl} \quad [6]
\]

where

- MM is mineral matter (% by mass)
- A is ash content (% by mass)
- P is pyritic sulphur in the coal (% by mass)
- CO2 is carbon dioxide that originates from the mineral matter in the coal (%)
- SO3 is sulphur trioxide in the ash (%)
- Cl is the chlorine in the coal (%).

**Representation of oxygen in coal**

South African coals have too high an oxygen content to be ignored for all calculations involving elemental analysis. In principle, representing the oxygen as O2, can be considered, or replacing some of the hydrogen or carbon of the coal to form compounds such as H2O, CO, or CO2. According to Powell (1945), free oxygen is present in coal gas only as a result of air leakage or introduction of air after the gas has left the carbonization chamber. Relatively small amounts of oxygen could also be associated with air originally present in the voldage between the coal particles plus that in the pores or adsorbed within the coal during charging. Therefore, from these considerations, assuming the coal oxygen to be O2 seems to be the least accurate assumption.

The Dulong formula (Rosenqvist, 1974) allows estimation of the gross CV of coal as calculated from the elemental analysis:

\[
\text{NCP} = 81 C + 340 (H - O/8) + 22 S \quad [7]
\]

where

- NCP is gross CV in kCal/kg (1 kCal = 4.184 kJ)
- C, H, O, and S are the mass percentages of these elements in an absolute dry coal sample.

Figure 1 – Oxygen contents of South-African coals and four imported hard coking coals (Schoeman and Boshoff, 1996)
The formula implies that oxygen decreases the contribution of hydrogen to the gross CV. This suggests that oxygen is combined with hydrogen in coal, probably as \( \text{H}_2\text{O} \), or at least the thermal effect thereof seems to be an acceptable approximation.

Several proposed molecular structures of coal have been published by various authors (Given, 1960; Wiser, 1973). If we consider a proposed structure of vitrinite, we observe that most oxygen is present in \( \text{C}–\text{O}–\text{H} \), less in \( \text{C}–\text{O}–\text{C} \) bonds, and some \( \text{C}=\text{O} \) bonds are also found (Shinn, 1984). From such a structure oxygen would not be liberated as \( \text{O}_2 \).

From the vitrinite structure in Figure 2, the coal would preferably be represented by a small number of species with less complex molecular structure and known thermodynamic properties. Even studying the type of bonds does not help much in suggesting which species would best represent oxygen in the coal. However, whatever species are chosen, the mass balance should be satisfied (it should reflect the elemental composition of the coal) and the energy balance should be satisfied. Potentially one could choose any one of \( \text{O}_2, \text{H}_2\text{O}, \text{CO}, \) or \( \text{CO}_2 \).

The effect of the choice of a compound to represent oxygen in coal on the results obtained is illustrated by the simple hypothetical ‘process’ in Figure 3. Table IV gives the assumed composition of the hypothetical coal used in this study. The hypothetical coal is simplified by assuming it is dry and the ash has only one constituent: \( \text{SiO}_2 \). One kilogram of this coal is oxidized with 2.25 kg oxygen to yield an off-

---

**Table III**

Proximate and ultimate analyses and calorific values of South African coals and four imported hard coking coals (Schoeman and Boshoff, 1996)

<table>
<thead>
<tr>
<th>Ultimate analysis (air-dry base), mass %</th>
<th>Gross CV, (air-dry base), MJ/kg</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>H</td>
</tr>
<tr>
<td>A</td>
<td>79.56</td>
</tr>
<tr>
<td>B</td>
<td>75.07</td>
</tr>
<tr>
<td>C</td>
<td>76.42</td>
</tr>
<tr>
<td>D</td>
<td>79.34</td>
</tr>
<tr>
<td>E</td>
<td>83.65</td>
</tr>
<tr>
<td>F</td>
<td>85.09</td>
</tr>
<tr>
<td>G</td>
<td>74.81</td>
</tr>
<tr>
<td>H</td>
<td>76.07</td>
</tr>
<tr>
<td>I</td>
<td>80.99</td>
</tr>
<tr>
<td>J</td>
<td>82.30</td>
</tr>
<tr>
<td>K</td>
<td>79.64</td>
</tr>
<tr>
<td>L</td>
<td>80.37</td>
</tr>
<tr>
<td>M</td>
<td>73.33</td>
</tr>
<tr>
<td>N</td>
<td>43.76</td>
</tr>
<tr>
<td>O</td>
<td>41.12</td>
</tr>
<tr>
<td>P</td>
<td>50.63</td>
</tr>
<tr>
<td>Q</td>
<td>70.10</td>
</tr>
<tr>
<td>R</td>
<td>72.38</td>
</tr>
<tr>
<td>S</td>
<td>71.90</td>
</tr>
<tr>
<td>T</td>
<td>75.35</td>
</tr>
<tr>
<td>U</td>
<td>54.92</td>
</tr>
<tr>
<td>V</td>
<td>59.07</td>
</tr>
<tr>
<td>W</td>
<td>71.31</td>
</tr>
<tr>
<td>X</td>
<td>70.79</td>
</tr>
<tr>
<td>Y</td>
<td>72.69</td>
</tr>
<tr>
<td>Z</td>
<td>70.17</td>
</tr>
<tr>
<td>AA</td>
<td>77.03</td>
</tr>
<tr>
<td>AB</td>
<td>69.42</td>
</tr>
<tr>
<td>AC</td>
<td>66.77</td>
</tr>
<tr>
<td>AD</td>
<td>66.40</td>
</tr>
<tr>
<td>AF</td>
<td>68.64</td>
</tr>
<tr>
<td>AG</td>
<td>61.78</td>
</tr>
<tr>
<td>AH</td>
<td>53.77</td>
</tr>
<tr>
<td>AI</td>
<td>67.78</td>
</tr>
<tr>
<td>AJ</td>
<td>69.20</td>
</tr>
<tr>
<td>AK</td>
<td>68.20</td>
</tr>
<tr>
<td>AL</td>
<td>70.29</td>
</tr>
<tr>
<td>AM</td>
<td>70.09</td>
</tr>
<tr>
<td>AN</td>
<td>56.19</td>
</tr>
<tr>
<td>AQ</td>
<td>69.29</td>
</tr>
<tr>
<td>AR</td>
<td>71.65</td>
</tr>
<tr>
<td>AS</td>
<td>71.80</td>
</tr>
<tr>
<td>AT</td>
<td>73.86</td>
</tr>
<tr>
<td>AU</td>
<td>70.44</td>
</tr>
<tr>
<td>AV</td>
<td>72.09</td>
</tr>
</tbody>
</table>
gas containing surplus O$_2$. The hypothetical heat load of the process is 25.00 MJ. The remaining heat is allocated to the flue-gas. The flue-gas temperature is calculated for different assumptions. Flue-gas temperatures were determined for coal oxygen represented as:

In principle, coal could be represented by a mixture of species, including oxygen-containing species other than those from list above. However, the list was chosen to illustrate a concept that could be applied to any valid selection of species. The Ex Mente™ Easy Thermo program was used to perform the equilibrium calculation.

Table V gives the resulting flue-gas temperatures from this study. For the four cases, the flue-gas temperature varied between 807°C and 1128°C, which suggest that the choice of...
Representation of coal and coal derivatives in process modelling

the compound to represent oxygen in coal has a significant influence on the accuracy of modelling.

From fundamental analysis of the problem, there are at least four different reasons why any representation of coal could be inaccurate as far as the energy balance is concerned.

➤ Amorphous carbon in coal is at a higher free energy as well as enthalpy state compared to graphite. This is illustrated in Figure 4. The difference of about 5 kcal/mole C (1 kcal = 4.184 kJ) equates to about 1.0 MJ/kg for coal containing 60% C, or up to about 1.5 MJ/kg for higher grade coals (having higher carbon content). Coke carbon is associated with a free energy state intermediate between coal and graphite. For modelling purposes, thermodynamic values for graphite are generally available and used.

➤ Depending on the assumption of how oxygen in the coal is represented, significant differences in calculated energy requirement or consumption for the same process could occur.

➤ Energy is required for liberation of the organic volatiles. However, this value is usually not known for a specific coal.

➤ Energy is consumed during pyrolysis of inorganic compounds such as clays and carbonates (associated with ‘inert volatiles’, as discussed).

For pyrometallurgical modelling involving solid carbon, as well as for tar, results from the bomb calorimeter can be used to calibrate the enthalpy balance. These results represent real behaviour, while calculated results could be inaccurate as previously explained. Such a calibration procedure should rectify inaccuracies resulting from all the reasons mentioned, including the choice of a compound to represent oxygen in coal.

It is hereby suggested that the calculated CV should be compared with the experimentally obtained CV, and the balance used as a correction for the enthalpy of the coal or coal derivative. In principle, this approach is also shared by Peacey and Davenport (1979) for the purpose of modelling the injection of coal and other hydrocarbons into a blast furnace. The balance between calculated CV and gross heat of combustion yields the heat of formation of a hydrocarbon from the elements. That indicates that the assumption is made of O₂ representing oxygen in coal, instead of e.g. H₂O(l) which, from the discussion above seems to be a more logical choice.

Subsequently, the effects of determining the correction value were studied for each of the four cases (where four different species were selected to represent oxygen in coal) to determine the effect of using each correction value on the predicted flue-gas temperature of the hypothetical process (see Table VI). The strategy involved calculating a coal enthalpy correction value as follows:

\[
\text{Coal enthalpy correction value} = \text{Gross CV} - \text{Calculated CV} \quad [8]
\]

The unit of this correction value would be MJ/kg. By adding the enthalpy correction value (which could be either positive or negative) to the calculated CV, the CV would be corrected to represent the experimentally determined gross CV. For the present hypothetical study, the coal enthalpy correction value was calculated for each of the four cases, where oxygen in the coal was represented by different species. Subsequently, the coal enthalpy (where carbon is assumed to be graphite by default) was corrected by the correction value, and the corrected flue gas temperatures were calculated (Table VI).

A different coal enthalpy correction value is obtained for every compound assumed to represent oxygen. However, the corrected off-gas temperature is the same for all the different assumptions, namely 1074°C. Since the values, including the coal CV, used in this example are hypothetical, this does not provide proof of which compound best represents oxygen in coal.

Clearly, whatever the choice of the compound to represent oxygen in coal, the correction value yields the same correct flue-gas temperature, as the correction value itself depends on the choice of a compound to represent oxygen.

---

Table VI

<table>
<thead>
<tr>
<th>Assumption 1: O₂</th>
<th>Assumption 2: H₂O</th>
<th>Assumption 3: CO</th>
<th>Assumption 4: CO₂</th>
</tr>
</thead>
<tbody>
<tr>
<td>Flue-gas temperature before correction, °C</td>
<td>1128</td>
<td>807</td>
<td>1006</td>
</tr>
<tr>
<td>Coal enthalpy correction value, MJ/kg coal</td>
<td>0.247</td>
<td>-1.183</td>
<td>-0.306</td>
</tr>
<tr>
<td>Flue-gas temperature after correction, °C</td>
<td>1074</td>
<td>1074</td>
<td>1074</td>
</tr>
</tbody>
</table>
Nevertheless, it seems important that the correction yields a relatively accurate result. One could refer to the correction term as the ‘energy of decomposition of the volatiles’. However, that would suggest that, after devolatilization, no correction term would be required, while the form of carbon (graphite vs. amorphous carbon or coke) is still of importance. To designate the correction term, ‘heat of formation of a hydrocarbon’ (the approach by Peacey and Davenport, 1979) would yield an accurate result. However, the representation of oxygen as O<sub>2</sub> could seem conflicting, as studies suggest that oxygen would not be liberated from coal as O<sub>2</sub> (except for minute quantities originating from the pores in the coal).

Although H–O bonds are not the only way oxygen is combined in coal (Figure 2), representing oxygen in coal by H<sub>2</sub>O(l) seems to be a logical choice. The question arises about the general accuracy of predicting the CV of South African coals by calculating from elemental analysis without using the correction procedure. Data for the same set of coals as for Figure 1 was used for this purpose. The theoretical CV was calculated by the following formula, which was derived from the heats of combustion of the species in this study:

\[ CV_{(\text{calc})} = 0.3276\%C + 1.4179\%H - 0.1787\%O + 0.0926\%S \]  

where

- \( CV_{(\text{calc})} \) is the calculated gross CV of the coal on an air-dry base (MJ/kg)
- \( \%C \): % carbon (air-dry base)
- \( \%H \): % hydrogen (air-dry base)
- \( \%O \): % oxygen (air-dry base)
- \( \%S \): % total sulphur (air-dry base).

Note that Equation [9] is not the result of multiple regression analysis. For the calculation it was assumed the oxygen in coal is present as H<sub>2</sub>O(l) and carbon is present as graphite, according to the results depicted in Figure 5. Generally, good agreement between calculated and actual gross CV for all the different coals was found. Nevertheless, percentage errors up to 2.9% were found for this set of coal analyses. In order to increase the accuracy of the energy balance so that it is equal to that obtained from the calorimetric technique, the enthalpy correction term must be utilized.

A positive coal enthalpy correction value could be interpreted from the effect of a carbon form with a higher enthalpy than graphite outweighing the effect of decomposition of the volatiles, and vice versa. The purpose of the correction value is to correct the predicted CV to a value equal to that determined in the bomb calorimeter. If the process being modelled involves coal derivatives like coke, char, or tar, it would be advisable to determine the gross CVs of those coal derivatives and calculate enthalpy correction values for them, to be incorporated in the respective energy balances.

It is important to note that, apart from the coal enthalpy correction term, no additional correction value, as suggested by Figure 4, should be used, as that would represent double-counting of effects, which would introduce an error in the calculation process.

Another study was undertaken on the present set of South African coals by representing coal oxygen as O<sub>2</sub> instead of H<sub>2</sub>O(l), according to Figure 6. This assumption causes the coal calorific values obtained for the Free State and Mpumalanga coals to be over-estimated. Similar studies for oxygen represented as CO or CO<sub>2</sub> were not included.

Note also that the study is limited to South African coals. It is possible that selecting a different compound to represent oxygen could lead to slightly more accurate predicted CVs for different coals. Nevertheless, the recommendation to determine the CV of the coal and coal derivatives and correct the enthalpy by comparison with the gross CV is a general one.

**Conclusions**

Coal proximate analysis should not be regarded as absolute; it could vary with several parameters, including heating rate. For modelling, the use of ultimate analysis should be considered a preferable option to proximate analysis, where, ‘fixed carbon’ and ‘volatiles’ are not defined in terms of chemical composition. Significant errors could be introduced...
if the larger molecules are neglected during calculation of the calorific value (CV) of coal gas (the gas liberated when coal is heated in the absence of oxygen).

For elemental analysis, the oxygen content (which is calculated by balance) should be checked to ensure it is within the expected range. For representation of sulphur in coal, one should be careful to avoid double-counting due to SO₃ in the ash analysis.

Potentially, oxygen in coal could be represented as O₂, H₂O, CO, or CO₂. However, use of some of these species without considering the experimentally determined gross CV introduces significant errors in the energy balance. If coal enthalpy is calculated from elemental analyses without correction, representation of coal oxygen as H₂O(l) gives reasonable accuracy (up to 2.9% error for a set of South African coals). Coal volatiles could be represented by a complex mixture of compounds, even using different oxygen-containing species other than the abovementioned four, provided the enthalpy is corrected.

It is recommended that an ‘enthalpy correction value’ is incorporated in energy balances involving combustion, devolatilization, or conversion of coal and coal derivatives, e.g. coke, char, or tar. That would imply that proximate analysis, elemental analysis, as well as the gross CV would be required for all solid or liquid coal-derived substances being modelled. No other correction due to the form of carbon being different than graphite should be used, as that would imply double-counting some effects.

References


Sonic injection into a PGM Peirce-Smith converter: CFD modelling and industrial trials


Synopsis
Peirce-Smith converters (PSCs) are extensively used in the copper, nickel, and platinum group metals industries. The typical converting operation involves lateral purging of air into molten matte through a bank of tuyeres. This blowing operation occurs at low pressure from the blowers, resulting in a bubbling regime that is considered inefficient from both a process and an energy utilization perspective. Inherent drawbacks also include recurrent tuyere blockage, tuyere punching, and low oxygen efficiency.

Western Platinum embarked on a full-scale industrial evaluation of generating a jetting regime by using sonic injection. Prior to industrial-scale tests, a numerical assessment to ascertain the feasibility of implementing sonic injection into a PSC was conducted. The work included flow characterization at high-pressure injection achieving sonic velocity at the tuyere exit. The 2D and 3D simulations of the three-phase system were carried out using the volume of fluid method together with the RKE turbulence model to account for the multiphase and turbulent nature of the flow.

This paper discusses the key findings in understanding plume extension, velocity distribution, shear wall stress analysis, and phase distribution characteristics in the system. Plant trials are also discussed with reference to the commercial aspects of a full-scale implementation of sonic injection in the smelter.

Keywords
Peirce-Smith converter, sonic injection, CFD modelling.

Introduction
Despite lengthy operational experience, understanding of the mode and principle of Peirce-Smith converter (PSC) operation has not changed significantly. Some modifications to the typical PSC have been adopted, one notable example being the Hoboken converter, which is fitted with a siphon that permits process gas collection without atmospheric dilution (Bustos et al., 1995). Hoefele and Brimacombe (1979) allude to historical conservatism, rather than technological limitations, as the reasons for resistance to change.

Small versions of copper-nickel PSCs are used in platinum group metals (PGMs) smelters for removing Fe and S chemically associated with Cu-Ni mattes rich in PGMs. Lonmin plc operates a PGM PSC approximately one-third the working volume of a typical copper-nickel PSC. Due to the bubbling regime resulting from subsonic flow conditions currently employed in these operations, common problems are encountered. These include tuyere blockages (which necessitate frequent punching operations); high refractory wear in the tuyere region; substantial splattering and splashing, which generate significant amounts of reverts (Richards et al., 1986; Wraith et al., 1994; Kapusta, 2010) and also cause operational downtime with intermittent off-stack periods for cleaning the converter mouth and aisle; and reduced oxygen efficiency, which is attributed to the punching operation as a result of substantial air losses due to leakages, limiting the converter capacity or the reprocessing of reverts and dusts. These process inefficiencies are accompanied by energy inefficiencies or ‘excess’ power consumption related to punching machines, leaks at the tuyere body due to punching (wasted blower air), and unreacted injected air.

The conversion process occurs in a high-temperature environment in a refractory-lined steel shell vessel, which precludes visual observation and experimentation. In order to delineate critical process parameters, physical and numerical modelling techniques have been developed. Physical models with different liquids simulating matte and slag have been developed to study gas plume, splashing, mixing, phase distribution, and mass transfer phenomena (Hoefele and Brimacombe, 1979; Richards et al., 1986; Chibwe, Akdogan, and Eksteen, 2011; Chibwe, Akdogan, Aldrich, and Eric, 2011; Chibwe, Akdogan, Aldrich, and...
Sonic injection into a PGM Peirce-Smith converter: CFD modelling and industrial trials

Taskinen, 2011). Richards et al., (1986) concluded that the main cause of splashing was the development and intensification of slopping resulting from the manifestation of a uninode wave. Their analysis showed that gas-liquid coupling increases with tuyere submergence depth, hence the reduction in splashing. For the small working volume PSC used in the PGM industry, tuyere submergence is shallow relative to that in Cu-Ni PSCs (Brimacombe et al., 1984). Any possible injection consideration in the small PSC should take this limitation into account.

PSC campaign life is dependent on the integrity and state of the refractory in the converter. Due to subsonic flow conditions, the refractory in the tuyere line has commonly been observed to deteriorate much faster than in the rest of the converter. Three mechanisms of refractory wear have been identified: chemical corrosion, thermal spalling, and mechanical wear (Gonzalez et al., 2007). Goni et al. (2006) quantitatively estimated that 35–65% of refractory wear in a PSC is due to chemical and thermomechanical processes. This type of refractory erosion is the result of a combination of gas dynamics in the proximity of the tuyere nozzle where high temperature gradients exist, and the punching operation, which generates mechanical shock.

Brimacombe et al. demonstrated at both the laboratory (Hoefele and Brimacombe, 1979; Brimacombe and Hoefele, 1980; Brimacombe et al., 1990) and plant scales (Brimacombe et al., 1984; Bustos et al., 1987) that sonic injection (jetting regime) into copper or nickel converters could reduce or eliminate the above-mentioned process and energy inefficiencies. In 1979, Hoefele and Brimacombe carried out the first experimental studies on sonic injection into a PSC using air-water, air-ZnCl₂, and air-Hg systems coupled with plant trials. Pressure measurements in both laboratory experiments and plant trials showed that only the air-mercury system had the same bubble frequency as the plant, indicating the importance of the gas–liquid density ratios on the dynamics of submerged injection processes. Strikingly improved penetration of gas into liquid was observed at sonic conditions. Subsequent plant trials with straight-bore tuyeres designed for sonic flow were conducted at the ASARCO smelter in the USA (Brimacombe et al., 1984), the Toyo Smelter in Japan (Kimura et al., 1986), and the Noranda and INCO copper smelters in Canada (Bustos et al., 1987). The salient points from the above work are as follows: the horizontal penetration force is relatively low compared to the buoyancy force exerted by the bath; the stability of the tuyere accretions formed depends on converting cycle; and punchless operation is possible at higher injection pressure. Based on the understanding of accretion formation and stability, coupled with the process benefits of sonic injection, the Air Liquide Shrouded Injector (ALSI) technology was developed (Bustos et al., 1995). With ALSI technology, air oxygen enrichments between 30% and 40% have been achieved without detrimental refractory erosion. Commercial implementation of ALSI technology was inaugurated at the Falconbridge smelter in Canada (Bustos et al., 1999) and later notable applications included the Thai Copper Industries smelter (Kapusta et al., 2007).

Lonmin is interested in implementing such technology on a commercial scale. Prior to implementation, key process aspects needed to be evaluated, amongst them slopping, splashing and mixing characteristics, refractory integrity, and the possible extent of air penetration into the bath in these relatively small converters with shallow tuyere submergence. A realistic presentation of such a system needed to be developed in order to obtain conclusive interpretations for initial trials. Moreover, a rigorous system development satisfying the geometry and dynamic similarity was also needed.

For this purpose, characterization of the dynamics of the three-phase (air, matte, and slag) flow in the PSC used at Lonmin was conducted at high air pressure injection achieving sonic velocity at the tuyere tip by using CFD simulations. The 2D and 3D simulations of the three-phase system were carried out using the volume of fluid (VOF) and realizability turbulence models to account for the multiphase and turbulent nature of the flow respectively. These models were implemented using the commercial CFD numerical code FLUENT. The simulations from the current investigation revealed both qualitative and quantitative results of flow characteristics in the converter, which paved the way forward in planning the trials and selecting the converter to equip with sonic tuyeres. The full-scale plant trials have been successfully completed with promising results.

Numerical simulations

In this work, 2D and 3D simulations were carried out based on a slice model of the Lonmin PSC. Table I gives the dimensions of the actual converter and slice model.

The computational domain was discretized into small control volumes for the calculations. Very fine meshes in the tuyere region were necessary to accurately capture the flow pattern. Domain decomposition was done in order to facilitate mesh multiple methods with local control for the creation of a conformal hybrid mesh as shown in Figure 1.

Modelling was done on an Intel® Core™ i7 CPU with 3.46 GHz processor and 8.0 GB installed random access memory (RAM). The commercial CFD code ANSYS FLUENT, version 14.0, was used for the calculations on a high-power computing (HPC) cluster with an installed capacity of eight 2.83 GHz processors per node with 16 GB of RAM. In this paper, simulations conducted at midway through a typical blow will be presented, as this period accounts for more than 85% of the converting cycle time. In order to reduce the computational time during the simulations, the flow in the sonic tuyere was not included but simulated separately, and the flow conditions at the tuyere exit were taken as the inlet boundary condition of the computational domain. This value was calculated using the isentropic flow theory. Only two

<table>
<thead>
<tr>
<th>Table 1 Lonmin converter and slice model dimensions</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dimensions</td>
</tr>
<tr>
<td>Diameter inside refractory (mm)</td>
</tr>
<tr>
<td>Length inside refractory (mm)</td>
</tr>
<tr>
<td>Tuyere inner diameter (mm)</td>
</tr>
<tr>
<td>Number of tuyeres</td>
</tr>
<tr>
<td>Average tuyere spacing (mm)</td>
</tr>
</tbody>
</table>
Simulations were conducted with a 300 mm tuyere pipe coupled to the converter to visualize the development of air flow into the converter. A segregated solver with an implicit approach was used to calculate the pressure, velocity, turbulence, and density through solving unsteady and compressible flow conservation-governing equations, namely continuity, momentum, and energy. In order to account for the multiphase nature of the flow, the VOF model was used. The interfacial behaviour of air, matte, and slag was captured by this model using a compressive discretization scheme. This is accomplished by surface tracking of the phase interfaces in the system through solution of the VOF continuity equation. In the model, the different phases are treated numerically as interpenetrating continua, thus inevitably introducing the concept of phasic volume fraction where the volume fractions in each computational cell sum to unity. The effects of turbulence on the flow field inside the model were incorporated by using the realizable k-ε model, which offers improvements in the overall energy transfer. The flow conservation-governing equations, the VOF equation, and turbulence model equations were solved with FLUENT version 14.0. This package is a finite-volume solver using body-fitted computational grids. A coupled algorithm was used for pressure-velocity coupling. A compressive interface capturing scheme for arbitrary meshes (CICSAM) discretization was used to obtain face fluxes when the computational cell is near the interface using a piecewise-linear approach. This scheme was necessary due to the high viscosity ratios involved in this flow problem (ANSYS, 2011). A time step of 0.0001 seconds was used and found to be sufficient for maintenance of numerical convergence at every time step and stability. Convergence of the numerical solution was determined based on surface monitoring of integrated quantities of bulk flow velocity and turbulence and scaled residuals of continuity, x-, y-, z- velocities. The residuals of all quantities were set to 0.001, and the solution was considered converged when all the residuals were less than or equal to the set value.

Results and discussion

CFD modelling

From the numerical simulations conducted in this work, the computed plume extension for current (subsonic) and envisaged sonic operation are plotted in Figure 2. A dimensionless parameter (x/de) where x is the exit jet distance (in millimetres) and de is the exit tuyere diameter (in millimetres) was used to visualize the extent of the plume penetration into the converter.

In Figure 2, the plume extension into the bath for subsonic and sonic conditions is indicated by ‘Plume Sonic’ and ‘Plume Subsonic’. According to these results, plume sonic penetration into the bath is four times longer than that of plume subsonic. The extension of the plume region into the converter away from the tuyere exit area is essential as it provides extra volume for chemical reactions to take place. In their mass transfer studies of the PSC, Adjei and Richards (1991) concluded that the substantial part of the chemical reactions in the converter is likely to occur in the tuyere plume region.

Also, the simulations reveal that the bath circulatory velocity outside the plume region is approximately 0.27 m.s⁻¹ for both flow conditions. These results are in consistent agreement with the assumption made by Bustos, Brimacombe, and Richards (1988) in their development of a mathematical model for accretions growth in PSCs for...
Sonic injection into a PGM Peirce-Smith converter: CFD modelling and industrial trials

Subsonic and sonic operations. Figure 3 shows the velocity vector distribution around the tuyere exit for both flow conditions. It can be observed that the sonic injection plume extends further into the bath, and with a higher velocity, than with subsonic operation. Lower velocity regions are evident further away from the plume.

Figure 4 shows the phase density distribution for subsonic and sonic flow conditions. A high air volume region in front of the tuyeres can be seen for sonic flow conditions, compared with subsonic flow. This is consistent with the results shown in Figures 2 and 3. Due to the agitation in the regions in front of the tuyeres, a strong emulsification exists, resulting in high reaction rates in the zone. This is in agreement with the observations by Rosales et al. (1999) in their study of fluid dynamics in a Teniente converter.

The effects of bath circulation and bath density on the walls of the converter were evaluated by calculating wall shear stress along the converter wall boundaries. Figure 5 shows the wall shear stress distribution for subsonic and sonic flow conditions. Near the tuyeres, for subsonic flow conditions a maximum wall shear stress of 200 Pa was obtained compared to 125 Pa for sonic flow. This suggests that sonic injection could reduce the refractory wear due to mechanical erosion around the tuyere region. At the wall opposite to the tuyeres line, the stress is higher for sonic injection due to the propagation of waves further from the tuyeres, which carry energy to the opposite sidewalls. This is desirable for achieving better mixing conditions in the converter, whereas with subsonic conditions energy is instantly dissipated just above the tuyeres as shown in Figure 3, which might lead to increased refractory erosion.

Plant trials

Plant trials were conducted to demonstrate the feasibility of high-pressure sonic injection technology into relatively small PSCs. Once the target total flow rate of compressed air into the converter and the number of sonic tuyeres had been finalized, sonic tuyeres were designed and dimensioned. All of the necessary equipment for the supply and control of the compressed air flow to the converter was also sourced in preparation for the trials. A new reline was installed and the punching machine was removed. The sonic tuyeres were installed using the same tuyere body as for normal operation. SCADA programming, alarms, and control set-points were then carefully evaluated and implemented to ensure the safe and controlled operation of the converter during the sonic injection trials.

The main purpose of high-pressure injection is the development of a different flow regime in the tuyere region through manipulation and designing of the blowing conditions and configuration. In this work, the dimensionless parameters – namely tuyere flow Mach number and injected air specific mixing power ($\varepsilon_m$) – were the main criteria for PSC manipulation and design for sonic injection. The injected air specific mixing power ($\varepsilon_m$) is given by:

$$\varepsilon_m = \varepsilon_b + \varepsilon_k$$  \[1\]

where $\varepsilon_b$ is the specific mixing power due to buoyancy and $\varepsilon_k$ the kinetic energy. The mathematical expressions are given in Equations [2] and [3]:

Figure 3 – Velocity vector distribution around the tuyere exit for (a) subsonic and (b) sonic flow conditions

Figure 4 – Phase distribution density contours for subsonic and sonic flow conditions

Figure 5 – Wall shear stress distribution for subsonic and sonic flow conditions
Sonic injection into a PGM Peirce-Smith converter: CFD modelling and industrial trials

\[ \varepsilon_b = \frac{2Q_p}{W} \ln \left( 1 + \frac{\rho_b H_s}{P_a} \right) \]  

where

- $W$ is the effective bath weight (kg)
- $Q$ is the total gas flow rate (Nm\(^3\)s\(^{-1}\))
- $P_a$ is the atmospheric pressure (kPa)
- $A$ is the total tuyere cross-sectional area (m\(^2\))
- $\rho_b$ is the bath density (kgm\(^{-3}\))
- $H_s$ is the injection submergence (m)

The PSC blowing conditions are given in Table II.

From Table II, it is evident that as the blowing conditions change from subsonic to sonic regime, the \(\varepsilon_b/\varepsilon_k\) ratio changes in such a manner that the flow is dominated by kinetic specific mixing power at sonic operation.

Before the sonic injection trials began it was found that the main characteristics of subsonic injection were the high variability of both the air flow rate and the injection pressure, as shown in Figure 6. This high variability is a direct consequence of the blocking accretions that form, resulting in lower flow and higher pressure, and the unplugging of the tuyeres by punching, resulting in a sudden higher flow and lower pressure.

In contrast, as shown in Figure 7, the air flow rate during sonic injection is less variable compared to subsonic injection. A more stable air flow rate is one of the expected benefits of sonic injection. The flow rate curve shows a significantly reduced variability compared to the blow shown in Figure 6. Even more significant is the stability of the sonic injection pressure. The stability of both the flow rate and pressure demonstrated that the new operating strategy was successful. Controlled splashing was also accompanied by a stable flow rate and pressure of compressed air, as illustrated in Figure 7. Also, the maximum refractory wear rate ranged between 10.3 and 11.1 mm per blow, which corresponds to 37 to 40 blows per campaign, or a 34% reduction in refractory wear compared with conventional subsonic injection. These measurements of refractory wear, although conducted over a short period of time or a short number of blows, still provide an industrial validation of the theory that the accretions formed during sonic injection are indeed protective rather than disruptive.

When operated in sonic mode, the converter capacity to reprocess reverts was found to increase by as much as 200% compared to the low-pressure bubbling regime, owing to the relatively higher oxygen efficiency. In summary, sonic injection offers significant flexibility for periods of high production of furnace matte – reducing the revert reprocessing rate to take full advantage of fast sonic blows – or for periods when a high reverts reprocessing capacity is needed. Table III highlights some of the benefits of using a sonic regime in the converter.

\[ \varepsilon_k = \frac{\rho_b Q^3}{2WA^2} \]

Table II

<table>
<thead>
<tr>
<th>PSC blowing conditions</th>
<th>Number of tuyeres</th>
<th>Tuyere internal diameter (mm)</th>
<th>Tuyere Mach number</th>
<th>(\varepsilon_k) (kWt(^{-1}))</th>
<th>(\varepsilon_b/\varepsilon_k)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Subsonic converter</td>
<td>18</td>
<td>48</td>
<td>0.32</td>
<td>6.73</td>
<td>4.87</td>
</tr>
<tr>
<td>Sonic converter</td>
<td>8</td>
<td>32</td>
<td>1.0</td>
<td>6.79</td>
<td>1.35</td>
</tr>
</tbody>
</table>

Table III

Comparison of sonic and subsonic trials at Lonmin

<table>
<thead>
<tr>
<th>Factors</th>
<th>Operation</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Subsonic (current)</td>
</tr>
<tr>
<td>Punching operation</td>
<td>Yes</td>
</tr>
<tr>
<td>Oxygen efficiency, %</td>
<td>65</td>
</tr>
<tr>
<td>Converter campaign, cycles</td>
<td>26</td>
</tr>
<tr>
<td>Scrap reprocessing, ton</td>
<td>2.97</td>
</tr>
<tr>
<td>In-stack time, min</td>
<td>469</td>
</tr>
</tbody>
</table>
Sonic injection into a PGM Peirce-Smith converter: CFD modelling and industrial trials

Conclusions
The CFD modelling formed part of an assessment to complement feasibility studies of implementing high-pressure sonic injection into relatively small Peirce-Smith converters (PSCs) used at Lonmin plc prior to the plant trials. The modelling work was carried out to characterize the fluid dynamics of three-phase (air, matte, and slag) fluid flow with high-pressure injection of air at sonic velocity. The modelling results provided a basis for further development of sonic injection into relatively small industrial PSCs, with the ultimate objective of reducing energy consumption, improving process efficiency, and increasing the throughput of the converting process. The results revealed that the plume extended into the bath approximately four times deeper at sonic flow conditions relative to subsonic flow conditions. Lower wall shear stress values for sonic flow conditions suggest that sonic injection could prolong the refractory life. Higher pressure injection gave rise to regions of high air volume in front of the tuyeres relative to low-pressure injection operation. With subsonic flow the injected gas ascended near the converter wall above the tuyeres for a significant period of time and thus a high refractory wear in the tuyere region would be expected relative to sonic injection. These findings showed that high-pressure injection into PGM PSCs converters is feasible.

Following the modelling exercise, sonic injection trials at one of Lonmin’s converters were successfully completed. Punchless operation was achieved with sonic injection, with the capacity to reprocess much larger amounts of reverts than when operating in the conventional mode due to the higher oxygen efficiency in sonic mode. Sonic injection resulted in a lower refractory wear per blow or per ton of matte, leading to longer campaign cycles.

In summary, sonic injection offers significant flexibility for Lonmin’s converting operation by allowing operators to adjust their practice for periods of high production of furnace matte – reducing the reverts reprocessing rate to take full advantage of fast sonic blow – or for periods when a high reverts reprocessing capacity is needed.

Acknowledgements
The authors acknowledge Lonmin Plc for the financing of this work, and express their gratitude to all personnel at Lonmin’s converter aise for their support and commitment to the success of the plant trials. Permission from BBA and Lonmin to publish this paper is also appreciated.

References
Physical and numerical modelling of a four-strand steelmaking tundish using flow analysis of different configurations

by J.H. Cloete*, G. Akdogan*, S.M. Bradshaw*, and D.K. Chibwe*

Synopsis
Modern tundishes have evolved as vessels to serve as the final step in refining of molten steel by removing inclusions and promoting thermo-chemical homogeneity.

In this study the flow behaviour in a four-strand tundish was investigated by means of a ½-scale water model as well as numerical modelling. The numerical and physical models were used to characterize residence time distribution and calculate properties pertaining to tundish flow regime. Three different tundish configurations were investigated: a bare tundish with no flow control devices, a tundish with a turbulence inhibitor, and a tundish with both a turbulence inhibitor and a dam.

The physical and numerical models showed that a tundish without flow control devices is prone to significant short-circuiting. A tundish with a turbulence inhibitor was shown to be successful in preventing short-circuiting and provided surface-directed flow that might assist the removal of inclusions from the melt. However, it was also observed that the upward-directed flow caused the maximum turbulence kinetic energy near the surface to increase dramatically. The potential for slag entrainment should therefore be considered during the design and operation of tundishes with turbulence inhibitors.

Keywords
tundish, steelmaking, CFD, physical modelling, numerical modelling.

Introduction
The metallurgical importance of tundishes has led to much research into various aspects of tundish operation and design, and investigations of the flow properties and inclusion behaviour through both physical and numerical modelling. A large portion of the research has been focused on the use of flow control devices to alter flow patterns and improve the tundish performance by eliminating short-circuiting, increasing the residence time to promote inclusion removal, and reducing variation between strands in multi-strand tundishes (Craig et al., 2001, 2003; Kumar et al., 2007, 2008; Jha et al., 2008; Tripathi and Ajmani, 2011; Zhong et al., 2007). Craig et al. (2001) worked on the optimization of a single-strand stainless steel caster tundish for two separate tundish configurations – dam and weir, and baffle with angled holes and an impact pad. Significant improvements of up to 34% in minimum residence time were obtained for the second configuration. Moreover, in 2003 Craig et al. reported a CFD study combined with mathematical optimization to design the configuration of the new enlarged tundish. Design variables chosen included the position and sizes of baffles and baffle holes and pouring box width, while the design objective was maximization of the minimum residence time (MRT) at operating level and at a typical transition level. The study showed that mathematical optimization techniques can be coupled with CFD techniques to obtain optimum tundish designs with significant improvements.

In general, most authors have assumed the tundish to be isothermal, but some have looked at the effect of temperature gradients due to heat loss from the tundish (Liu et al., 2008; Mishra et al., 2012; Miki and Thomas, 1999) or the effect of the cooling rate of melt arriving from the ladle (Qu et al., 2012). Modelling strategies are necessary when investigating tundish behaviour because of the high temperature and opaque nature of the steelmaking process, which makes performing certain experiments on the real system impossible. For the physical modelling procedure, full- or reduced-scale water models, based on Reynolds number or Froude number similarity, are used (Mazumdar and Guthrie, 1999). The flow behaviour is usually characterized by investigating the residence time distribution (RTD) curves under various operating and design parameters.

In this study a physical model was used to investigate the effect of different turbulence inhibitor designs on the flow properties of a four-strand trough-shaped tundish to contribute to the current knowledge and
Physical and numerical modelling of a four-strand steelmaking tundish

understanding of multi-strand tundish design and operation. Of specific interest is a design proposed by Kumar et al. (2008) where the use of a turbulence inhibitor with holes in combination with low dams is proposed to improve flow properties. This study investigated whether the addition of the holes and dams provides significant advantage compared with using only a turbulence inhibitor without holes, which would be less expensive to construct and maintain. A numerical model was also developed in FLUENT to simulate the flow behaviour in the water model, improving the understanding of the results of the physical model experiments. The effect of the assumptions of symmetry and dynamically steady flow on numerical results, which were frequently used in tundish CFD studies to reduce the computational time (Kumar et al., 2008; Tripathi and Ajmani, 2011; Zhong et al., 2007; Mishra et al., 2012; Tripathi and Ajmani, 2005; Jha et al., 2001) was also investigated. This is of importance, as there is no information on the effects of these assumptions on computational accuracy in the available literature on tundishes. The numerical model was also used to investigate the effect of the upward flow on surface turbulence, since high surface turbulence creates the potential for slag entrainment, which will cause new inclusions to form and lower the product quality. This is therefore a factor worth considering when implementing the use of turbulence inhibitors.

Experimental modelling

The physical model was constructed from clear, 6 mm PVC, with all dimensions scaled to a 1:2 ratio compared to the industrial tundish. The four sidewalls were inclined by 10°. The dimensions of the tundish are shown in Figure 1.

The turbulence inhibitor was constructed from grey PVC, 15 mm thick. The dimensions are shown in Figure 2. The turbulence inhibitor was attached to the tank using silicone adhesive, when required for experiments. The holes in the side of the turbulence inhibitor could be closed by inserting correctly sized PVC blocks into them and sealing the gaps with silicone.

The complete physical model set-up is shown in Figure 3. To simplify construction, the water feed tank was placed to the side of the tundish model. However, CFD simulations showed that by simply placing a 90° bend in the feed pipe above the tundish, an asymmetric velocity profile would develop. To rectify this, an 8 litre cubic tank, made from stainless steel, was suspended above the inlet point at the centre of the tundish. CFD simulations showed that this ensures an even velocity profile in the inlet pipe. The inlet pipe had a diameter of 30 mm and penetrated the tundish to 165 mm from the bottom of the tundish. A T-junction at the top of the inlet pipe allowed tracer fluid to be injected into the inlet stream using a syringe. Outlet holes were drilled in the bottom of the bath. The desired flow rate, at the bath height used, was obtained by calculating the required diameter of the outlet from Bernoulli’s equation. A PVC insert with the correct diameter was then placed into each of the holes. The measured flow rates in each of the outlets were within 2% of the desired rate. Apart from geometric similarity, the Froude number was used as the criterion for dynamic similarity. In reduced-scale water modelling it is impossible to simultaneously achieve both Froude number and Reynolds number similarity. It has been shown by Sahai and Emi (1996) that the RTD response of tundish water models is insensitive to the Froude number over a large range of values, and to the Reynolds number, if the tundish is operated in the turbulent regime. Since tundishes are generally operated turbulently, either Froude number or Reynolds number similarity may be used to scale the flow rates for the water model. However, Froude number (Equation 1) similarity is required for the modelling of inclusions and is therefore most often used in tundish physical modelling. In this study, Froude number similarity was selected to enable addition of inclusions to the water model in the future.

Table I gives a comparison of design and operating parameters for the industrial tundish and the 1:2 water models. During scaling based on the Froude number, the inlet flow rate of the water model was calculated so that the Froude number at the inlet is identical to that of the industrial tundish. The Froude number at the inlet is calculated as:

\[ F_r = \frac{v^2}{gd} \]  

[1]
During the experiments, the water was first allowed to run for approximately 15 minutes at the desired flow rate to allow a steady flow to develop in the tundish model. An aqueous potassium chloride solution (200 g/l) was used as tracer. To initialize the experiment 50 ml of the tracer solution was injected near the inlet. This was done over a period of five seconds to prevent the tracer injection from disturbing the inlet velocity profile to a significant extent. The delay this caused was justified by the fact that for all set-ups, except for the bare tundish, the minimum residence times are relatively large compared to this delay.

For the duration of the experiment the total dissolved solids in the water passing through an outlet was monitored using a conductivity meter. The conductivity meter was placed in a small container below the outlet to prevent disturbance of the flow pattern within the tundish. The volume of the container was minimized to allow the delay caused by the mixing to be small compared to the residence times observed. The experiment was performed for only two of the outlets, because of the symmetry of the geometry. Five experiments were performed for each tundish configuration to obtain an average residence time distribution that accounts for variation between runs.

### Flow characterization

Several properties were calculated from the RTD results of both the physical and numerical experiments to characterize the flow in the tundish being studied. The first step was to derive the dimensionless C-curve for the tundish. The dimensionless time, \( \theta \), was calculated as:

\[
\theta = \frac{t}{t_\text{mean}}
\]  

where \( t \) is the theoretical mean residence time, \( \tau = \frac{V}{Q} \)

The dimensionless concentration of strand \( i \) (the outflow at outlet \( i \)) can be calculated as:

\[
C_i = \frac{c_i V}{M}
\]

where \( V \) is the total volume of the tundish, \( c_i \) the concentration in the strand, and \( M \) the total amount of tracer injected.

Since the flow rates in all strands are equal, the overall dimensionless concentration can be simply calculated as the average of the individual strand concentrations. Another important characteristic property of the flow is the mean residence time, \( t_\text{mean} \), calculated as:

\[
t_\text{mean} = \frac{\int C(t) dt}{\int C(t) dt}
\]

To calculate the mean residence time for an individual strand, the average concentration at the outlets, \( C \), is simply substituted by the concentration at the strand being considered. The tundish performance can further be classified by dividing the tundish into three flow volumes: the plug volume (\( V_p \)), the well-mixed volume (\( V_m \)), and the dead volume (\( V_d \)), which are defined according to the modified combined model by Ahuja and Sahai (1986) as:

### Table I

<table>
<thead>
<tr>
<th>Property</th>
<th>Industrial tundish</th>
<th>Water model</th>
</tr>
</thead>
<tbody>
<tr>
<td>Length (m)</td>
<td>3</td>
<td>1.5</td>
</tr>
<tr>
<td>Volume (l)</td>
<td>2000</td>
<td>250</td>
</tr>
<tr>
<td>Mass flow rate (kg/min)</td>
<td>1015</td>
<td>25.6</td>
</tr>
<tr>
<td>Volumetric flow rate (l/min)</td>
<td>145</td>
<td>25.6</td>
</tr>
<tr>
<td>Bath height (m)</td>
<td>0.78</td>
<td>0.39</td>
</tr>
<tr>
<td>Froude number</td>
<td>1.24</td>
<td>1.24</td>
</tr>
</tbody>
</table>
Physical and numerical modelling of a four-strand steelmaking tundish

\[ V_o = \frac{1}{2} (\theta_{\text{min}} + \theta_{\text{mean}}) \]  

[6]

\[ V_d = 1 - \frac{Q_d}{Q} \times \theta_{\text{mean}} \]  

[7]

\[ V_w = 1 - V_o - V_d \]  

[8]

The ratio \( \frac{Q_d}{Q} \) is the fractional volumetric flow rate through the active region and is equal to the area under the C-curve between the bounds of \( \theta = 0 \) and \( \theta = 2 \). After \( \theta = 2 \), the tail data is considered to be only from the dead regions.

Numerical modelling

Numerical simulation has several advantages over physical modelling. Firstly, it provides information on properties throughout the flow domain. Therefore, information regarding the velocity and turbulence kinetic energy profiles can be used to explain the RTD results obtained through physical modelling and to identify possible ways to improve the system. Secondly, once an accurate model has been developed, different geometries can easily be studied using the numerical model without making costly and time-consuming changes to a physical model. In this study the commercial CFD package FLUENT® 14.5 was used. A review of the literature on tundish numerical modelling (Chattopadhyay et al., 2010) showed that the majority of authors had used the standard k-\( \varepsilon \) model to model turbulence. The standard k-\( \varepsilon \) turbulence model has been shown to be reasonably accurate in predicting flow characteristics for a single-strand tundish from RTD experiments, and is still preferred above slightly more accurate models because of significantly lower computational times (Jha et al., 2003). For this study the realizable k-\( \varepsilon \) (RKE) model was selected since it provides additional accuracy for swirling flows and is only slightly more computationally expensive than the standard k-\( \varepsilon \) model.

At the inlet, the normal velocity, calculated from the inlet area and the volumetric flow rate, was specified, assuming a flat profile at the ladle outlet. The top surface of the model was assumed to be flat and frictionless. This was done by declaring the surface as a wall with zero shear stress components in all three dimensions. The outlets were specified as pressure outlets with zero gauge pressure. The combination of the bath height and outlet diameter caused the total outlet mass flow to be equal to the inlet mass flow rate. All other surfaces were set to stationary walls, assuming the no-slip condition. The standard wall function was used to model the turbulence near the walls. The flow was assumed to be symmetrical over the planes through the centre of the bath along its length and its width, hence a quarter model was used. Therefore, zero gradients of all properties were assumed normal to these planes. The three-dimensional geometry of the fluid volume was created for the different geometries considered in this study and meshed using a tetrahedral mesh. The mesh was refined near curved walls and walls with close proximity to each other to produce a mesh of acceptable quality. Figure 4 shows the domain modelled with CFD.

In FLUENT, the flow and turbulence in the domain was first solved for steady flow, reaching a converged solution after approximately 12 000 iterations. For the final simulations, this initial solution was then used to locally refine the mesh in areas with high velocity gradients, using the gradient adaption function in FLUENT to obtain a more accurate solution. Throughout this study the minimum mesh orthogonal quality, a measure of the mesh quality, was maintained above 0.09 after gradient adaption. General guidelines suggest not using meshes with a minimum orthogonal quality of less than 0.05 (ANSYS, 2011); therefore sufficient mesh quality is maintained in this study. The final meshes contained approximately 2.8 million cells. The refined mesh was then used to solve for more accurate flow and turbulence solutions, requiring approximately 15 000 additional iterations for a converged solution. The transient and species solvers were then activated and the momentum and turbulence solvers turned off. This allowed the transient movement of the tracer fluid to be tracked in the steady velocity and turbulence fields. To simulate the physical experiment, the inlet boundary condition was set to add tracer to the tundish for five seconds, after which the addition of tracer was stopped. The concentration of tracer at the outlets was then monitored for two and a half times the theoretical mean residence time of the tundish to calculate the flow characteristic properties from the RTD response.

Grid independence and validation

A grid-independence study was performed to determine whether the mesh used is sufficient to accurately solve the flow in the tundish. This was done by repeating the numerical experiment for cases with different specified mesh sizes and comparing the RTD curves. A mesh specified with a constant size is preferred, since this is the easiest to set up and to use in different geometries. However, due to the contrast between the fast flow near the inlet and outlets and the very slow flow through the rest of the bath, the gradients in the bath will also vary to a large extent. For this reason, some areas will require a very fine mesh for accurate
solutions, while most of the tundish will require only a coarse mesh. Therefore, by refining the mesh in regions with high velocity and turbulence gradients, a more efficient numerical model can be obtained. It was determined that grid independence was achieved by performing a single refinement, using the gradient adaption tool in FLUENT, on a 10 mm mesh, effectively reducing the size of the adapted cells to 5 mm. The velocity gradient at which adaption starts was determined by lowering the adaption threshold until the final solution no longer changed appreciably.

Results and discussion
In this study, aspects of the modelling procedure, such as symmetry, steady flow, and grid independence, were investigated. Next, the numerical model was validated against physical model results for three different configurations. The first set-up consisted of a bare tundish; therefore no flow control devices were used. The second set-up used a combination of the turbulence inhibitor with holes (TID), shown in Figure 2, and a low dam, which altered the flow by forcing it over the dam. The ratio of the dam height to the bath height was 0.2. The dam was placed at \( X = 0.39 L \) where \( X \) is the distance from the inlet to the dam and \( L \) is half the length of the tundish. The final set up included a turbulence inhibitor, as shown in Figure 2, but with the side holes closed (TI). This allows the effect of the inclusion of the holes and dams, the design proposed by Kumar et al. (2008), to be evaluated. Finally, the numerical model results were used to evaluate the performance of the different tundish configurations.

Symmetry assumption
The geometry of the tundish used in this study is symmetrical over two planes. Using this knowledge, the fluid volume solved in FLUENT can be reduced to a quarter of its original size, reducing the computational time required significantly. Another simplification to the numerical model that is frequently used in tundish modelling is to assume dynamically steady flow. This assumption allows only the species equation, which converges much faster than the momentum and turbulence equations, to be solved transiently. This allows a single iteration per time step to be used, instead of approximately six to eight iterations per time step, drastically reducing the required computational time.

Although both of these assumptions are frequently used in tundish literature (Kumar et al., 2008; Tripathi and Ajmani, 2011; Zhong et al., 2007; Mishra et al., 2012; Tripathi and Ajmani, 2005; Jha et al., 2001), there is little information available about their effect on the numerical results. For this reason, the RTD curves were compared for three different cases: dynamically steady flow with two symmetry planes, dynamically steady flow without symmetry, and fully transient flow without symmetry. The tundish configuration used for the comparison was the turbulence inhibitor with holes in combination with the dams. However, because of the high computational requirements of the cases without simplifying assumptions, it was clear from preliminary grid-independence results that these solutions would not be feasible with the amount of cells required to reach grid independence. Hence a mesh of 14 mm cells was used for this comparative study to allow a rough estimate of the effect of these assumptions. The results shown use an average value of three simulations for each case, to account for variability in the results. The variability was much higher than for the final grid-independent runs. It was argued that this was because a new mesh was generated for each run, causing differing numerical errors due to the mesh being insufficiently fine in certain areas.

Figure 5 shows that the use of two symmetry planes does have an effect by slightly increasing the peak concentration. However, from knowledge gained from further grid investigations, it was seen that the effect of accurately resolving the mesh is much more important than solving the full geometry. Therefore, the use of the symmetry assumption is justified by the fact that it allowed the use of a finer mesh for a more accurate solution within acceptable computational time. It was therefore decided to use the model applying both symmetry planes and dynamically steady flow and focus on obtaining a more accurate grid-independent solution.

Flow characteristics
The characteristic flow quantities calculated from the physical and numerical experiments are summarized in Table II. Additionally, the RTD curves for the numerical solution for the three cases are shown in Figure 6.
It can therefore be concluded that the numerical model is acceptable for predicting the flow properties of different tundish configurations. This is particularly the case when considering the assumptions employed to reduce the computational time: symmetry, dynamically steady flow, and a flat, frictionless surface.

A numerical simulation was also performed for the case of a turbulence inhibitor with high dams (TIHD), where the height of the dams was increased by 50% over the TID case. Comparison of the flow characteristic properties in Table II shows that the higher dam is in fact able to prevent the short-circuiting in the system, since the value of the dimensionless minimum residence time increases from 0.043 to 0.084. Unfortunately, this improvement comes with a cost, as the peak residence time is significantly reduced and the dead volume is increased slightly. The likely reason for this deterioration of the flow quality is that the higher dam causes larger dead volumes between the turbulence inhibitor and the dams, as well as behind the dams.

It is observed that the minimum residence time for the TID case is less than half of that observed for the TI case. Therefore, a fraction of the flow will spend a very short time in the tundish, allowing larger inclusions to reach the outlet without being removed. In conclusion, it can therefore be stated that there does not appear to be any clear evidence that the use of holes and dams, in combination with a turbulence inhibitor, offers any significant benefit over using only the turbulence inhibitor.

The short minimum residence time for the TID case is most likely due to the dams being too low to completely eliminate short-circuiting of the flow passing through the holes. It was suggested that it might be possible to eliminate this problem by increasing the height of the dams. Industrial trials would be required to determine whether the prevention of large inclusions passing through by short-circuiting in the TID case is worth the reduction in peak residence time and increase in the dead volume when the height of the dams is increased. However, the TI case still performs better, without the added complication and cost of more complex flow control devices.

As a final matter of interest, the amount of turbulence predicted near the surface by the numerical model was investigated for the bare, TI, and TID cases. The magnitude of the turbulence near the tundish surface is very important due to the potential of slag entrainment. From previous discussions it is also obvious that the addition of the turbulence inhibitor influences the flow near the surface to a

<table>
<thead>
<tr>
<th>Set-up</th>
<th>Data source</th>
<th>$\theta_{\min}$</th>
<th>$\theta_{\text{peak}}$</th>
<th>$\theta_{\text{mean}}$</th>
<th>$V_p$</th>
<th>$V_d$</th>
<th>$V_m$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bare</td>
<td>Physical</td>
<td>0.0101</td>
<td>0.0670</td>
<td>0.687</td>
<td>0.039</td>
<td>0.370</td>
<td>0.591</td>
</tr>
<tr>
<td></td>
<td>Numerical</td>
<td>0.0077</td>
<td>0.0732</td>
<td>0.705</td>
<td>0.040</td>
<td>0.375</td>
<td>0.585</td>
</tr>
<tr>
<td></td>
<td>% difference</td>
<td>27.5</td>
<td>8.84</td>
<td>2.64</td>
<td>4.76</td>
<td>1.19</td>
<td>1.08</td>
</tr>
<tr>
<td>TI</td>
<td>Physical</td>
<td>0.089</td>
<td>0.234</td>
<td>0.756</td>
<td>0.162</td>
<td>0.306</td>
<td>0.532</td>
</tr>
<tr>
<td></td>
<td>Numerical</td>
<td>0.091</td>
<td>0.298</td>
<td>0.784</td>
<td>0.196</td>
<td>0.278</td>
<td>0.526</td>
</tr>
<tr>
<td></td>
<td>% difference</td>
<td>1.89</td>
<td>24.1</td>
<td>3.22</td>
<td>18.5</td>
<td>16.1</td>
<td>13.15</td>
</tr>
<tr>
<td>TID</td>
<td>Physical</td>
<td>0.035</td>
<td>0.291</td>
<td>0.747</td>
<td>0.163</td>
<td>0.299</td>
<td>0.538</td>
</tr>
<tr>
<td></td>
<td>Numerical</td>
<td>0.043</td>
<td>0.326</td>
<td>0.790</td>
<td>0.184</td>
<td>0.259</td>
<td>0.557</td>
</tr>
<tr>
<td></td>
<td>% difference</td>
<td>18.7</td>
<td>11.3</td>
<td>5.81</td>
<td>12.2</td>
<td>14.4</td>
<td>3.48</td>
</tr>
<tr>
<td>TIHD</td>
<td>Numerical</td>
<td>0.084</td>
<td>0.279</td>
<td>0.764</td>
<td>0.181</td>
<td>0.279</td>
<td>0.540</td>
</tr>
</tbody>
</table>

It is immediately apparent from the results that the introduction of the turbulence inhibitor offers advantages over the use of the bare tundish, as reported by Kumar et al. (2008). This is due to the fact that the turbulence inhibitor prevents short-circuiting along the bottom of the tundish by forcing upward flow. This leads to a significant increase in the minimum, peak, and mean residence times. Since sufficient time is necessary for the flotation of inclusions by buoyant forces to the slag, these increased residence times enable more inclusions to be absorbed by the slag layer. The result is that the number and size of non-metallic inclusions in the steel product will be reduced, providing a product of higher quality and value. Additionally, the higher plug flow volume fraction will provide less turbulent flow, which promotes the rising of the inclusions in the melt, while the decreased dead volume enhances thermal and chemical homogeneity in the product. Also, the upward-directed flow will help to bring the inclusions into contact with the slag for absorption. However, the primary purpose of this study was to evaluate the benefit of including holes and low dams to the turbulence inhibitor. The purpose of the holes is to accelerate upward flow away from the inlet region, thereby helping to eliminate dead volumes.

Comparing RTD results for the physical and numerical experiments using the adapted mesh in Table II, a good correlation was reached for the calculated flow characteristics. The average difference in the properties calculated for the three different configurations is approximately 10%. The largest difference, recorded for the breakthrough time in the bare model, is easily explained by the delays in input and measurement in the physical model, which become significant for the very short minimum time. The other value where large differences are detected is the peak time for the cases using a turbulence inhibitor. The numerical model predicts longer times for the peak concentration to be reached, which in turn translates into larger plug flow volumes and lower dead volumes. What is of importance is that despite these differences, general trends between the different configurations are the same for the physical and numerical model. The numerical model predicts the much lower breakthrough time due to short-circuiting in the bare set-up, as well as the small amount of short-circuiting for the case with the turbulence inhibitor with holes. Also, the bare tundish clearly has much lower plug flow and larger dead volumes than the configurations using turbulence inhibitors. It can therefore be concluded that the numerical model is...
large extent by introducing upward flow in the inlet region. It is therefore necessary to evaluate the effect of the upward flow on surface turbulence, because entrainment due to increased turbulence may offset any benefits of longer residence times and increased plug flow gained by the addition of the turbulence inhibitor. It should be noted that without a separate study to determine the dependency of slag entrainment on turbulence conditions, the discussion regarding entrainment in this study is qualitative in nature. Nevertheless, the changes in flow along the longitudinal symmetry plane can be observed in Figure 7, and it can be seen that the upward-directed flow away from the inlet does increase. Comparing the turbulence kinetic energy values on a plane 2 cm below the surface of the tundish in Figure 8, it can be seen that the turbulence inhibitor changes the nature of the surface turbulence significantly. Firstly, it is noted that

Figure 7 – Comparison of velocity vector plots along the longitudinal symmetry plane for (a) the TI configuration and (b) the TID configuration

Figure 8 – Comparison of turbulence kinetic energy value near the surface of the tundish for (a) the bare tundish, (b) the TI configuration, and (c) the TID configuration
regions with slightly more turbulence develop at the far end from the inlet in all three configurations due to a circulation formed at the surface after flow is turned back at the back wall. However, this discussion will focus on the area near the inlet, where more surface turbulence occurs. In the bare tundish a high-turbulence region is formed near the sidewalls close to the inlet due to the flow rising along the walls. When the turbulence inhibitor is introduced, the high-turbulence region is centred on the inlet due to the rising flow from the turbulence inhibitor. It is important to note that the maximum value of turbulence (2.17×10^{-4} \text{ m}^2/\text{s}^2) is significantly increased from the bare case (9.67×10^{-5} \text{ m}^2/\text{s}^2). It is therefore recommended that surface turbulence should be considered when changing the design of a tundish to include a turbulence inhibitor. It would be valuable to study whether the turbulence generated near the surface would be sufficient to entrain slag droplets, either by physical or numerical modelling.

Visual comparison between the TI and TID cases in Figure 8 shows that the areas of higher turbulence expand very slightly with the addition of the holes and dams, with the average turbulence kinetic energy increasing from 6.01×10^{-5} \text{ m}^2/\text{s}^2 to 6.49×10^{-5} \text{ m}^2/\text{s}^2. The most likely explanation for this increase is that due to the increased strength of the circulation pattern at the top of the tundish for the TID case, more turbulence is generated when the flow rising from the inlet joins the flow from this circulation pattern.

Conclusions
A reduced-scale water model of a four-strand tundish was developed. The model was then used to perform RTD experiments to determine the flow behaviour of three different tundish configurations: a bare tundish with no flow control devices, a tundish with a turbulence inhibitor, and a tundish with both a turbulence inhibitor and a dam. A numerical model was also developed to simulate the behaviour of the water model to gain a clearer understanding of the physical model results. The numerical model was successfully validated against the physical model results.

A bare tundish was proven to be insufficient in providing good flow properties for tundish operation. Short minimum, peak, and mean residence times will limit inclusion removal, while a lack of strand similarity will reduce the quality of the product. High dead volumes will also prevent adequate mixing for homogenization and low plug flow volumes will limit inclusion removal. Both configurations with turbulence inhibitors were shown to decrease short-circuiting, decrease the dead volume, increase the plug flow volume, and increase the mean residence time. However, the addition of holes and dams to the configuration with only a turbulence inhibitor shows no clear improvement in flow properties. In fact, short-circuiting of the fluid passing through the holes decreases the minimum residence time and will allow larger inclusion to reach the mould. This short-circuiting could be prevented by increasing the height of the dams, but this approach resulted in a lower peak residence time and slightly larger dead volumes. It was determined that the surface-directed flow caused by the turbulence inhibitor more than doubles the maximum turbulence kinetic energy near the surface of the melt, increasing the potential for slag entrainment. The surface turbulence should therefore be considered during turbulence inhibitor design.

Acknowledgements
The authors wish to acknowledge NRF bursary funding for H. Cloete.

References


Modelling of fluid flow phenomena in Peirce-Smith copper converters and analysis of combined blowing concept

by D.K. Chibwe*, G. Akdogan*, P. Taskinen†, and J.J. Eksteen*‡

Synopsis
This investigation consists of a numerical and physical modelling exercise on flow patterns, mixing, solid-liquid mass transfer, and slag-matte phase distribution in a 0.2-scale cold model of an industrial Peirce-Smith converter (PSC). Water, kerosene, air, and sintered benzoic acid compacts were used to simulate matte, slag, injected gas, and solid additions into the PSC. The 2D and 3D numerical simulations were carried out using volume of fluid (VOF) and realizable k-ε (RKE) turbulence models to account for the multiphase and turbulence nature of the flow respectively. These models were implemented using the commercial computational fluid dynamics numerical code FLUENT.

Numerical and physical simulations were able to predict, in agreement, the mixing and dispersion characteristics of the system in relation to various blowing conditions. Measurement of mass transfer indicated that fluid flow in the PSC is stratified. Blowing configurations and slag volume both had significant effects on mixing propagation, wave formation, and splashing.

As a potential process alternative to increase conversion efficiency, we propose a combined blowing configuration using top lance and lateral nozzles. The numerical simulations were conducted on combined as well as lateral blowing conditions, and the results of the combined concept are encouraging.

Keywords
Peirce-Smith converter, combined blowing, CFD, mixing, splashing.

Introduction
Peirce-Smith converters (PSCs) have been used in the copper and PGM smelting industries for more than a century for the purpose of removing iron and sulphur through oxidation reactions to obtain blister copper and converter matte respectively. This process step is referred to as conversion (Liow and Gray 1990; Real et al., 2007). The conversion process used in removing iron and sulphur from matte is a complex phenomenon involving phase interactions, many chemical reactions, associated heat generation, as well as product formation (Kyllo and Richards, 1998a). The PSC is a cylindrical horizontal reactor (circular canal geometry) where air at subsonic velocity (Mach < 1) is injected into matte through submerged lateral tuyeres along the axis of the converter (Gonzalez et al., 2008). The converting process is semi-continuous and autothermal. Since there are chemical reactions taking place with products being formed, quality and quantity of mixing are important.

Mixing promotes chemical reactions, removing the products from reaction sites, and minimizes temperature and the composition inhomogeneities caused by cold solid additions in the form of scrap, process ladle skulls, reverts, and fluxes, which are inherent to the converting processes. Due to generation of turbulence in the converter, mixing may also aid inclusion agglomeration, coalescence, and flotation of impurities, thus improving converter efficiencies (Gray et al., 1984).

Mixing is important in submerged pyrometallurgical gas injection systems and has attracted much attention. Most research on mixing and injection phenomena in gas/liquid multiphase systems has been conducted for steelmaking and ladle metallurgy (Castillejos and Brimacombe, 1987; Kim and Fruehan, 1987; Sahai and Guthrie, 1982; Sinha and McNallan, 1985; Stapurewicz and Themelis, 1987). Turkoglu and Farouk (1991) defined mixing intensity and efficiency in terms of the time required to achieve a well-mixed bath – which is the time required, after the introduction of tracer, for tracer concentration at every nodal location in the system to reach a value that varies by no more than ±5% .

Despite substantial PSC operational experience, there has been insufficient research on the process engineering aspects. Mixing and mass transfer in the converter are key process parameters that have been studied very little. Due to the similarity of the basic concepts in ladle injection and the PSC, the core tenets of the work on ladle injection have...
been adopted in research into process characterization of the PSC in an effort to address the challenges in productivity (Gray et al., 1984; Hoefe and Brimacombe, 1979; Vaarno et al., 1998). Physical and numerical models of the PSC have been developed to study multiphase fluid flow phenomena (Liow and Gray, 1990; Koohi et al., 2007; Valencia et al., 2004). These models have been used in pyrometallurgical operations to establish functional relationships of process variables such as reaction kinetics (Kyllo and Richards, 1998b), injection dynamics (Schwarz, et al., 2001), and fluid flow behavior (Han et al., 2001; Real et al., 2007; Valencia et al., 2004). Despite the amount of numerical and experimental work on the fundamental phenomenon of multiphase flow, little effort has been addressed to the understanding of the combined effect of blowing rates and the presence of a slag phase on the overall mixing performance of the converter. If proper mixing is not achieved in the reactor, the fundamental consequences are chemical, thermal, and particulate inhomogeneities, resulting in undesirable variability in the final product composition.

PSC process reactions are highly exothermic in nature and high temperatures can result, depending on the grade of charged matte. It has become common practice to add cold flux and scrap, process reverts, and ladle skims in order to control the thermodynamics of the process. The solid-liquid mass transfer step may play an important role in the process performance and attainment of thermal and chemical bath homogeneity. The mechanism of dissolution of the cold additions and behaviour of active sites within the converter are not well understood. Rates of dissolution can be assumed to affect the thermal state of the converter and hence to be a factor that affects the turnaround time of the converter processing. Establishing a stable functional state of the converter, and fully developed categorization of flow fields, is therefore necessary for effective process control.

As mentioned above, the literature pertaining to solid-liquid mass transfer in ladle metallurgy is fairly comprehensive. Despite this, no in-depth studies have been found that address this critical subject of solid-liquid interactions in PSCs. The only source close to the subject is the study by Adjei and Richards (1991), who investigated gas-phase mass transfer in a PSC using a physical model. Their work revealed pertinent information relating to oxygen utilization efficiency in the converter.

In the PSC, the injected air has two main functions, which are to supply oxidant and energy to stir the bath. Energy is supplied in three forms, namely kinetic, buoyancy, and expansion. Energy and oxidant supply affect the chemical and physical processes in the converter such as converting rate, oxygen efficiency, dispersion of matte and slag, mixing, heat and mass transfer, slopping, splashing, and accretion growth (Haida and Brimacombe, 1985; Valencia et al., 2004). Again, little effort has been addressed to the understanding of the complex phase interactions of the three-phase system in terms of volumetric dispersion in relation to the flow conditions presented by tuyere-specific power. Dispersion is a subject that needs further understanding as substantial amounts of valuable metal are lost due to entrainment; a situation that leads to the incorporation of slag-cleaning systems in copper production circuits (Moreno et al., 1998; Warczok et al., 2004).

In this work, firstly the dependence of mixing on volumetric air flow rate and simulated slag quantities for different matte and slag levels is investigated using a combination of physical and numerical modelling. Secondly, we aimed at monitoring different regions in the PSC for solid-liquid mass transfer analysis. This was carried out through calculation of the localized turbulence characteristic and mass transfer coefficient. The dependence of these two mass transfer parameters on operating system variables such as air flow rate and the presence of a second phase (slag) were investigated. Thirdly, we investigated the effect of volumetric gas flow rate in the dispersion and interaction of matte and slag phases in the PSC.

Due to the scarcity of quantitative research work to date on PSCs, an overall strategy was devised to explain and evaluate experimental results using numerical simulation of the converter through computational fluid dynamics (CFD) software. Vaarno et al. (1998) and Valencia et al. (2004) evaluated the applicability of mathematical formulation to the PSC process using cold model experiments and established velocity vector fields. In similar studies, Vaarno et al. (1998) and Valencia et al. (2004) investigated the influence of the Froude number on bath mixing, jet stability, and splashing in a PSC using mathematical formulation and cold model experiments. This work presents a first attempt to study the dispersion and interaction of phases in the PSC.

In order to attain our physical modelling objectives, a 0.2-scale water bath physical model with equivalent properties to the generic industrial PSC used in copper smelters was designed using similarity principles. Geometric, dynamic, and kinematic similarity criteria were used in the design for equivalency between prototype and model, since hydrodynamic studies on fluid flow are not concerned with thermal and chemical similarity effects (Mazumdar, 1990). The modified Froude number, which represents fluid flow dominated by inertial and gravitational forces, was used for dynamic similarity. The molten liquid phases in the real PSC (matte and slag) were simulated in the model with water and kerosene respectively due to kinematic similarity.

In support of the physical modelling work, we also used isothermal transient multiphase 2D and 3D CFD numerical simulations. The CFD numerical code FLUENT software was used to solve the transient Navier-Stokes equations. The realizable k−ε turbulent model and volume of fluid (VOF) method were used to model the turbulence nature and multiphase flow respectively.

Experimental methods

Physical model description

The physical experiments for mixing, mass transfer, and phase dispersion measurements were conducted in a 0.2-scale PVC water bath model as shown in Figure 1. A polyvinyl chloride 2.5 inch cylindrical manifold served as a reservoir for compressed air at a constant line pressure supply of 5.5 bar. An inline VFlowMate digital mass flow meter, which uses the thermal mass flow principle, was used to measure the volumetric flow rate of compressed air into the model. The flow meter was powered with a low-voltage
Modelling of fluid flow phenomena in Peirce-Smith copper converters

limited current power source. This water model also formed the basis for the numerical simulations.

Similarity using dimensionless numbers is the key feature in the development of physical models. In the design process, geometry, kinematic, and dynamic similarities were observed through consideration of dimensionless numbers. Geometric similarity was observed using a scale factor on all physical dimensions, and dynamic similarity achieved through the modified Froude number, \( N_{Fr} \), which resembles fluid flow dominated by inertial and gravitational forces. Kinematic similarity was observed between the PSC and model through the Morton number, \( N_{Mo} \), which incorporates surface tensions, viscosities, and densities of the fluids. Modified Froude and Morton numbers are given in Equations [1] and [2] respectively:

\[
N_{Fr}^* = \frac{v_t^* \rho_l}{\rho_l(d_{o} - d_{w})g} [1]
\]

\[
N_{Mo} = \frac{g h^*}{\rho l \sigma} [2]
\]

where \( v_t \) (m s\(^{-1}\)) is the tuyere tip exit velocity, \( \rho_l \) (kg m\(^{-3}\)) is the liquid density, \( \rho_g \) (kg m\(^{-3}\)) is the gas density, \( g \) (m s\(^{-2}\)) is the gravitational acceleration, \( d_{o} \) (m) is the tuyere diameter, \( \mu \) (Pa s) is the dynamic viscosity, and \( \sigma \) (N m\(^{-1}\)) is the surface tension of liquid.

The condition of similarities yielded the dimensions, blowing conditions, and fluid physical properties as summarized in Table I.

For mixing time measurements, a tracer dispersion technique was used where sulphuric acid was injected in the centre of the model at 100 mm below the water (simulated matte) level and monitored by a pH meter placed directly opposite the tracer injection point at 100 mm from the converter circular wall. The midpoint of the bath was taken as the tracer injection point for simulation of the converter inputs charging point, which is situated in the centre of an industrial PSC. Figure 1 shows the tracer and pH meter positioning as used in this experimental set-up. Water was filled to a total constant height of 270 mm, which is 39% filling capacity. Kerosene was used to simulate the slag layer.

The kerosene-to-water height ratio was varied from 0% to 40% at five equidistant intervals. Air volumetric flow rate was varied from 0.00875 to 0.01375 N m\(^3\) s\(^{-1}\), which represents a typical scaled-down industrial operation range. A matrix of 25 experiments was designed and each experiment was repeated five times under the same conditions. An average mixing time was taken, which was within 10% standard deviation on all experimental conditions. The response was defined as the time taken to achieve uniform and homogeneous steady-state concentration of the bath after introducing a tracer. Decay in pH concentration to a value ±0.01 pH units represented 99% mixing in this work. In the numerical simulations for mixing time measurements, a region was adapted in the same location as the tracer injection point in the physical experiments where acid was patched with a volume fraction of 1. A custom field function was formulated at the position analogous to the pH position, measuring the mole fraction of tracer species concentration as a function of flow time. This was achieved through solving the species transport equation. Mixing was considered complete when the species concentration reached a stable value.

For solid-liquid mass transfer experiments, the benzoic acid cylindrical samples were 81 mm long and 38 mm diameter on average. To promote radial dissolution and minimize the end effects, the samples were enclosed between two thin mild steel washers on both ends. The benzoic acid compacts were mounted to a steel grid fastened with threaded rod. A total of eight samples were inserted in the converter model at a predetermined depth for every experimental run, as shown in Figure 2. The sample labelling convention used here shows sample number and submergence referenced from the converter bottom. Due to the shallow matte depth relative to the sample lengths, only two sample depths were considered in these experiments, namely 50 mm (H50) and 90 mm (H90) from converter bottom respectively. The samples were introduced and immersed into the water bath after the air volumetric flow rate had reached a steady-state value within ±1% of the required value and the simulated slag thickness had been added. The samples were simulta-

### Table I

<table>
<thead>
<tr>
<th>Similarity</th>
<th>Dimension</th>
<th>Industrial PSC</th>
<th>Model</th>
</tr>
</thead>
<tbody>
<tr>
<td>Geometric</td>
<td>Converter length (mm)</td>
<td>9140</td>
<td>1000</td>
</tr>
<tr>
<td></td>
<td>Converter inner diameter (mm)</td>
<td>3480</td>
<td>690</td>
</tr>
<tr>
<td>Dynamic</td>
<td>Number of tuyeres</td>
<td>42</td>
<td>7</td>
</tr>
<tr>
<td></td>
<td>Volumetric flow rate (N m(^3) s(^{-1}))</td>
<td>7.55</td>
<td>0.0113</td>
</tr>
<tr>
<td></td>
<td>Tuyere air velocity (m s(^{-1}))</td>
<td>138.5</td>
<td>30</td>
</tr>
<tr>
<td>Dynamic viscosity (Pa s)</td>
<td>12.45</td>
<td>12.45</td>
<td></td>
</tr>
<tr>
<td>Kinematic</td>
<td>Kinematic viscosity (m(^2) s(^{-1}))</td>
<td>0.01 (matte)</td>
<td>0.0009</td>
</tr>
<tr>
<td></td>
<td>Liquid density (kg m(^{-3}))</td>
<td>4600</td>
<td>1000</td>
</tr>
<tr>
<td></td>
<td>Surface tension (N m(^{-1}))</td>
<td>0.93</td>
<td>0.0728</td>
</tr>
<tr>
<td></td>
<td>Slag density (kg m(^{-3}))</td>
<td>3300</td>
<td>774</td>
</tr>
<tr>
<td></td>
<td>Slag/ matte density ratio</td>
<td>0.717</td>
<td>0.775</td>
</tr>
<tr>
<td></td>
<td>Morton number</td>
<td>2.65 × 10-11</td>
<td>2.65 × 10-11</td>
</tr>
<tr>
<td></td>
<td>Operating temperature (K)</td>
<td>1473</td>
<td>293</td>
</tr>
</tbody>
</table>

![Figure 1 – Schematic view of 0.2-scale water bath model showing tracer and pH probe arrangement as used in the mixing experiments](image-url)
Modelling of fluid flow phenomena in Peirce-Smith copper converters

...neously subjected to four cycles of 900 seconds’ treatment, during which they were removed at intervals, thoroughly dried, and weighed. The weight loss was converted into equivalent radii so as to calculate mass transfer coefficients. The air flow rates varied from 0.0025 to 0.01125 N m³ s⁻¹. Two simulated slag thicknesses, 54 mm and 108 mm, were used in the experiments, representing 20% and 40% of simulated matte height respectively. These two simulated slag volumes will be referred to as ‘low simulated slag’ and ‘high simulated slag’ volumes in the text.

In the phase dispersion measurements, the physical model was filled with water and kerosene to a total height of 285 mm, which is 41% filling capacity. The kerosene-to-water height ratio was kept at 0.267. Air volumetric flow rate was varied from 0.0085 to 0.0142 N m³ s⁻¹ with five levels representing 75, 90, 100, 110, and 125% of the typical equivalency model volumetric flow rate of 0.0113 N m³ s⁻¹. For a specific experimental set-up run, at the end of experiment all syringes positioned at relevant sampling points as shown in Figure 3 were pulled at once and the contents were poured into measuring cylinders. The emulsion in the measuring cylinders were given sufficient time for complete phase separation, and the volumes of water and kerosene were read directly. Dispersed phase hold-up was calculated as the volumetric percentage of slag or matte with respect to the total volume of emulsion at a certain plane. On average, 20 ml of emulsion per sampling point was taken for every run.

**Numerical model description**

2D and 3D numerical simulations were carried out based on the 0.2-scale water slice model of a PSC. The computational domain was discretized into small control surfaces/volumes (for 2D/3D) for the calculations. Very fine meshes are necessary to capture accurately the flow pattern. In this work, a multi-size variable mesh was used. Fine mesh elements were employed in the matte-slag domain with the free air region having elements approximately three times larger. Modelling was done on an Intel® Core™ i7 CPU with 3.46 GHz processor and 8.0 GB installed RAM. The commercial CFD code ANSYS FLUENT, version 13.0, was used for the calculations on a high-performance computing (HPC) cluster with an installed capacity of eight 2.83 GHz processors per node with 16 GB of RAM. The 2D and 3D domain computational grids were made up of 26 492 Map/Pave quad and 313 529 hexahedral elements respectively. About 99.97% and 98.86% for 2D and 3D elements respectively had an equisize skewness of less than 0.4, which translate to good mesh quality, necessary for an accurate and converged solution.

**Figure 2** – Benzoic acid samples and top and side view of the spatial placements in the converter model

**Figure 3** – Schematic side view of model showing sampling depths
Modelling of fluid flow phenomena in Peirce-Smith copper converters

In order to account for the multiphase nature of the flow, the VOF model was used. The interfacial behaviour of air, matte, and slag was captured by this model using a compressive discretization scheme. This is accomplished by surface tracking of the phase interfaces in the system through solution of the VOF continuity equation. In the model, the different phases are treated numerically as interpenetrating continua, thus inevitably introducing the concept of phasic volume fraction where the volume fractions in each computational cell sums to unity. The effects of turbulence on the flow field inside the model were incorporated by using the realizable k-ε (RKE) model.

The flow conservation governing equations, the VOF equation, and turbulence model equations were solved with FLUENT version 13.0. This package is a finite volume solver using body-fitted computational grids. A coupled algorithm was used for pressure-velocity coupling. A Compressive Interface Capturing Scheme for Arbitrary Meshes (CICSAM) discretization was used to obtain face fluxes when the computational cell is near the interface, using a piecewise-linear approach. This scheme was necessary due to the high viscosity ratios involved in this flow problem. A time step of 0.0001 seconds was used and found to be sufficient for maintenance of numerical convergence at every time step and stability. Convergence of the numerical solution was determined based on surface monitoring of integrated quantities of bulk flow velocity and turbulence, and scaled residuals of continuity, x-, y-, and z-velocities, k, and ε. The residuals of all quantities were set to 0.001 and the solution was considered converged when all the residuals were less than or equal to the set value.

In the numerical simulations for mixing time measurements, a region was adapted in the same location as the tracer injection point in the physical experiments where acid was patched with a volume fraction of 1. A custom field function was formulated at the position analogous to the pH probe position, measuring the mole fraction of tracer species concentration as a function of flow time through solving the species transport equation. Mixing was considered complete when the species concentration reached a stable value. For a relatively thick simulated slag layer, the mixing time increased with an increase in the specific power of mixing; this is consistent with the results obtained by Valencia et al. (2004), who reported that an increase in air power generated more turbulence in the converter, with little benefit in terms of mixing quality in the mean flow of the bath. Figure 4 shows turbulence kinetic energy vector plots obtained in our study for air flow rates of 0.01125 N m$^3$ s$^{-1}$ and 0.01375 N m$^3$ s$^{-1}$ at constant slag thickness of 54 mm. It is evident from Figure 4(b) that at high blowing rates, high turbulence is created and concentrated in the tuyere region, as compared to low blowing rates shown in Figure 4(a). This phenomenon results in longer mixing times for the high slag thickness, but slightly shorter mixing times for low slag thickness, as shown in Figure 5.

From the results of the physical experiments, mixing time in terms of total specific mixing power (buoyancy plus gas kinetic energy) was analysed for 27 mm and 108 mm simulated slag thicknesses representing low slag and high slag operations respectively (Figure 5). The shorter mixing times obtained for low slag thickness and longer mixing times for higher slag thickness are attributed to the generation of increased turbulence in the converter, with little benefit in terms of mixing quality in the mean flow of the bath liquid.

Numerical simulations revealed that with thin simulated slag thicknesses, the slag is pushed to the opposite side of the tuyere line with the plume region being composed of almost only matte, as shown in Figure 6(a). This increases hydrodynamic pressure to the rising bubbles and hence increases the specific energy dissipated to the liquid phase for bath recirculation. This is due to high bubble retention in the liquid, which in turn increases mixing efficiency. However, the benefits of such retention time are offset by the effects of phase interaction, friction, and diffusion, which dissipate a substantial amount of energy at high slag volumes. The

Results and discussion

Mixing

Mixing time was found to decrease with increasing specific mixing power for the cases with thin simulated slag thickness. For a relatively thick simulated slag layer, the mixing time increased with an increase in the specific power of mixing; this is consistent with the results obtained by Valencia et al. (2004), who reported that an increase in air power generated more turbulence in the converter, with little benefit in terms of mixing quality in the mean flow of the bath. Figure 4 shows turbulence kinetic energy vector plots obtained in our study for air flow rates of 0.01125 N m$^3$ s$^{-1}$ and 0.01375 N m$^3$ s$^{-1}$ at constant slag thickness of 54 mm. It is evident from Figure 4(b) that at high blowing rates, high turbulence is created and concentrated in the tuyere region, as compared to low blowing rates shown in Figure 4(a). This phenomenon results in longer mixing times for the high slag thickness, but slightly shorter mixing times for low slag thickness, as shown in Figure 5.

From the results of the physical experiments, mixing time in terms of total specific mixing power (buoyancy plus gas kinetic energy) was analysed for 27 mm and 108 mm simulated slag thicknesses representing low slag and high slag operations respectively (Figure 5). The shorter mixing times obtained for low slag thickness and longer mixing times for higher slag thickness are attributed to the generation of increased turbulence in the converter, with little benefit in terms of mixing quality in the mean flow of the bath liquid.

Numerical simulations revealed that with thin simulated slag thicknesses, the slag is pushed to the opposite side of the tuyere line with the plume region being composed of almost only matte, as shown in Figure 6(a). This increases hydrodynamic pressure to the rising bubbles and hence increases the specific energy dissipated to the liquid phase for bath recirculation. This is due to high bubble retention in the liquid, which in turn increases mixing efficiency. However, the benefits of such retention time are offset by the effects of phase interaction, friction, and diffusion, which dissipate a substantial amount of energy at high slag volumes. The

Figure – 4 Turbulence kinetic energy vector plots for (a) 0.01125 N m$^3$ s$^{-1}$ and (b) 0.01375 N m$^3$ s$^{-1}$ air flow rate with 54 mm slag thickness
Modelling of fluid flow phenomena in Peirce-Smith copper converters

Mechanism of momentum transfer at simulated matte (simulated) slag-air interfaces fritters away potential recirculation energy. At an increased simulated slag thickness of 108 mm, as can be seen in Figure 6(b), the effect of interaction and dispersion is highly pronounced. As such, mixing in the simulated matte phase is expected to decrease. The effectiveness of the interphase exchange momentum is also reduced due to dissipation of energy by the simulated slag as a result of localized secondary recirculation flow, which is more pronounced at high simulated slag volumes. This observation is in agreement with the results reported by Han et al. (2001) on flow characteristics of a gas-stirred ladle model.

As indicated by Turkoglu and Farouk (1991), liquid bulk circulation rate is inversely proportional to mixing time, which indicates that the bulk motion of the liquid plays an important role in mixing, and hence that liquid recirculation rate can be used as a measure of mixing efficiency. Figure 7 shows the variation of average bulk velocity and turbulence kinetic energy with simulated slag thickness. Average bulk velocity and turbulent kinetic energy were calculated as the averages in infinite sampling points in the simulated matte calculation domain. It can be seen from Figure 7 that at 54 mm simulated slag thickness and above, the bulk recirculation velocity is greatly reduced. Moreover, turbulence was observed to decrease with increasing simulated slag height. Both these factors translate into increased mixing time.

In an effort to understand whether increased mixing time in the multiphase system was due to phase interactions, mixing time numerical simulations were also conducted with equivalent heights of matte only and matte plus simulated slag, of which simulated slag was 108 mm. Numerical simulations with only simulated matte depth displayed improved mixing efficiency, as shown in Figure 8, where mixing time is seen to decrease from 168 seconds (with slag) to 153 seconds (no slag). This could be attributed to improved momentum transfer between gas bubbles and the bulk liquid due to a high gas retention time, as well as the absence of energy dissipation in recirculation flow, and hence increased mixing efficiencies.

It is possible to postulate that when the melt height in the PSC is generally low, the gas channels through the melt along the vertical sidewall of the tuyere injection nozzle axis. In that case, the residence time of the gas bubbles in the melt is reduced, which in turn will reduce gas-melt interactions within the bulk melt. Therefore, as a result of channelling, the effectiveness of the gas momentum and power transfer to the bulk liquid flow is reduced. This adversely affects the mixing, liquid-liquid, and liquid-solid mass transfer within the bath. On the other hand, with an increase in liquid height in the converter, the axial plume residence time increases, which results in improved interaction between the gas and liquid. This will lead to more matte entrainment into the rising plume and a stronger agitation in the bath. In order to maintain consistent mixing power and offset the adverse conditions due to increased volumes of rising liquids, the bath height with respect to matte and slag ratio should be monitored in order to make necessary adjustments to the gas blowing rates for energy-efficient processing.

Solid-liquid mass transfer

Pyrometallurgical processes are multiphase in nature, involving gas-liquid-solid interactions. In PSC operation, the
addition of cold solids to the liquid matte in the form of fluxing agents (silica sands) for slag liquidity and process scrap and reverts for temperature control is a common practice. It is reasonable to propose that with such practice, the solid-liquid mass transfer step may play an important role in the performance of the process and attainment of liquid bath homogeneity. In this work, solid additions were simulated with sintered benzoic acid compacts spatially positioned in the model converter. Water and kerosene were used to simulate matte and slag respectively. Solid-liquid mass transfer was characterized by experimentally determined mass transfer coefficient values for benzoic acid sintered compacts and calculated dimensionless turbulence characteristic values. Two simulated slag thicknesses, 54 mm and 108 mm, were used in the experiments, representing 20% and 40% of simulated matte height respectively. These two simulated slag volumes will be referred to as ‘low’ and ‘high’ simulated slag.

The experimental results revealed that the dissolution varied with respect to all air flow rates and simulated slag volumes considered in this study. In Figure 9, S2 lies in the same location as S3 with respect to tuyere position but close to the simulated slag-matte interface. The dissolution rate was higher at S2 than at S3. On the other hand, sample S6, which is also near the simulated slag-matte interface, exhibited the second-highest dissolution rate ahead of S5. These observations indicate that there exists a circulatory and stratified flow regime in which the velocity flow variable differs with respect to the depth of the samples in the simulated liquids. This observation is consistent with earlier work by Vaarno et al., (1998), who measured experimentally and numerically liquid velocity distributions in a water model of a PSC. Their study identified a circulatory flow field in the converter with higher velocities near the bath surface. In the current work, this phenomenon is further attested to by the behaviour of S7 and S8, with S8 experiencing higher dissolution rates than S7. S1 and S4 also confirmed flow stratification, with higher dissolution being experienced at S4, which is near the slag-matte interface. It is also instructive to notice that both S1 and S4 had lower dissolution rates compared to S2, S3, S5, and S6. This observation serves to highlight that S1 and S4 are positioned in dead zones near the converter sidewalls in the model.

Two trends of dissolution behaviour were observed in terms of $K$ values as a function of simulated slag thickness and air flow rate. With low slag thickness, as air flow rate increased from 0.00875 N m$^3$ s$^{-1}$ to 0.01122 N m$^3$ s$^{-1}$, $K$ increased, then decreased towards 0.01375 N m$^3$ s$^{-1}$ but still remained higher than at 0.00875 N m$^3$ s$^{-1}$, as shown in Figure 10. This is possibly due to an increase in the fragmented body forces between the sample and emulsion, which increases the transport process as air flow rate increases. However, the observed decrease in mass transfer values as the air flow is increased further to 0.01375 N m$^3$ s$^{-1}$ is possibly due to shallow submergence of the tuyeres, with channelling phenomena becoming prevalent at high air flow rates (Adjei and Richards, 1991). Channelling will cause a breakdown of energy transfer to the system, hence a reduction in the transport process which results in the observed decrease in transport variable.

With high simulated slag thicknesses, and hence high slag volumes (Figure 11), we observed a decrease in values...
Modelling of fluid flow phenomena in Peirce-Smith copper converters

of \( K \) as air flow was increased from 0.00875 N m\(^3\) s\(^{-1}\) to 0.01122 N m\(^3\) s\(^{-1}\). It is possible that at these high slag volumes, phase interactions and interphase friction are strongly pronounced – so much so that fragmented body forces between the sample and emulsion are weakened, thereby retarding the transport process. A noticeable increase in the mass transfer parameters was observed with an increase in air flow to 0.01375 N m\(^3\) s\(^{-1}\). This could be a result of increased energy input to the system, the situation being sustained by slightly deeper tuyere submergence caused by the high slag volume, which allows for effective exchange of momentum between air and liquid. With the above facts in mind, it should be noted that the mass transfer values are still lower than those at 0.01122 N m\(^3\) s\(^{-1}\) with a low slag thickness (Figure 10). This scenario depicts under-utilization of capacity in terms of energy at high simulated slag volumes.

**Phase dispersion**

Experimentally measured dispersed phase holdup (Dph) at different planes in the water bath (Figure 12) was verified numerically with contours of volume fraction (VF) of simulated matte in simulated slag and simulated slag in simulated matte phase in the S and A planes respectively at 0.0113 N m\(^3\) s\(^{-1}\) (Figure 13). The results revealed that the amount of dispersed simulated matte in simulated slag phase in the model increases with increasing air volumetric flow rate. Conversely, it has been observed that the average amount of dispersed simulated slag in matte decreases. This situation could be attributable to the effects of increased splashing in the converter as air volumetric flow rate increases. According to Koohi *et al.* (2008), the splashes in the PSC are mainly matte constituents as slag is pushed to the radial position (Figure 6) opposite the tuyere side, forming a plume of matte. Splashes will disperse the matte out of the converter and those with insufficient kinetic energy will fall back onto the slag in the bath, resulting in increased matte entrapment in the slag layer (Figure 13, S-plane).
Numerical analysis of combined top and lateral blowing

As discussed in the previous sections, typical current operation of lateral-blown PSCs results in the common phenomenon of splashing and slopping due to air injection. The splashing and wave motion in the converter causes metal losses and potential lost production time due to the necessity for intermittent cleaning of the converter mouth, and thus reduced process throughput. Against such background, the purpose of this section is to report simulation results of combined blowing in a PSC using CFD and to compare the results of mixing propagation, turbulent kinetic energy, and splashing with the conventional common practice. This was done by creating four different sliced PSC models. The first two models represent the conventional practice, with tuyeres located at a lateral position on the converter. The slag layer thickness will be different for these two models, representing low and high slag volumes. The other two models also have dissimilar slag layer heights, but in these cases air will be injected from a combined top and lateral position.

Understanding the effect of combined top and lateral blowing could help identify whether combined top and lateral blowing is feasible for industrial usage, and possibly lead to alternative technologies for increased process efficiency in industrial PSCs.

In this work, 2D and 3D simulations were carried out based on slice models of a typical industrial copper PSC. Due to the mesh densities involved in these simulations, simulation of the entire converter was not feasible. Table II gives the dimensions, parameters for tuyere configurations, and bath (matte and slag) heights of the four different slice models based on the typical industrial converter considered in this study. LS1, LS2, CS1, and CS2 refer to lateral (L) blowing and combined (C) blowing models with low slag thickness (S1) and high slag thickness (S2) respectively. The dimensions and blowing parameters used correspond to those commonly employed in industry for lateral-blown PSCs. The velocity of the top-blowing air was taken to be the same as that for the lateral-injected air, as the aim of the study is to observe the effects of different locations of blowing and variance in slag layer height, and not the effects of inlet velocity.

The position of the top-blown lance above the molten liquids in the converter is very important. In the present investigation, the height and alignment of the top-blowing lance were selected after considering different sources in the literature regarding the position of lances for molten baths. For instance, Marcuson et al. (1993) mentioned that the lance was susceptible to degradation and recommend a lance height of 400 mm above the molten bath to ensure a high gas velocity at impact. In this study, the top-blowing lance was positioned 500 mm above the matte.

The flow conservation governing equations, the VOF equation, and turbulence model equations were solved with FLUENT version 14.0. A Semi-Implicit Method for Pressure-Linked Equation (SIMPLE) algorithm was used for pressure-velocity coupling. A Compressive Interface Capturing Scheme for Arbitrary Meshes (CICSAM) discretization method was used to obtain face fluxes, with a piecewise-linear approach. This scheme was necessary due to the high viscosity ratios involved in this flow problem (ANSYS, 2011). A time step of 0.0001 seconds was used and was found to be sufficient for maintenance of numerical convergence and stability at every time step. Convergence of the numerical solution was determined based on surface monitoring of integrated quantities of bulk flow velocity, turbulence, and scaled residuals of continuity such as the x-, y-, z-velocity components, \( k \), and \( \varepsilon \). The residuals of all quantities were set to \( 1\times10^{-3} \) and the solution was considered converged when all the residuals were less than or equal to the set value.
Modelling of fluid flow phenomena in Peirce-Smith copper converters

The solutions for the numerical simulations, based on density contour distribution of the liquids, are given in Figure 14 for the four models developed. In the analysis of these isosurfaces created in the middle of the models normal to the z-direction, it can qualitatively be observed that spitting and splashing originate from the tuyere side of the converter in all cases. This is due to the rupture of large bubbles generated from the tuyeres as they exit the liquid bath at the liquid surface. In the process, stable waves are created with slag being pushed to the sidewalls opposite the tuyere, leaving a plume generally consisting of matte phase.

It was also observed that there is an increase in matte velocity with combined blowing at high slag conditions, indicating the critical influence of lance height for combined blowing. In contrast, at high slag volume (272 mm slag thickness), it can be observed in Figure 14(b) that the air from the top lance has a pronounced effect on the wave path, creating a vortex on impact with the bath surface. In this instance, the distance from tuyere tip to bath surface is approximately 364 mm. This observation is consistent with the recommendation by Marcuson et al. (1993) for optimal lance tip to bath surface distance.

Turbulence kinetic energy distribution in gas-stirred systems is one of the important parameters influencing the mixing efficiency. It can be seen from Figure 15(a) that the addition of top-lance blowing increases the turbulence kinetic energy in the converter free space above the liquid. In the liquid bath, turbulence kinetic energy remains relatively the same, and thus we expect a similar overall oxidation rate in the two systems under consideration. However, it could be reasoned that the increased turbulence kinetic energy in the converter free space could speed up the fall of splash droplets back to the liquid bath surface. To further illustrate the effect of slag thickness, and thus the importance of tuyere tip-bath surface distance, velocity vector plots for 136 mm (S1) and 272 mm (S2) slag thickness are shown in Figure 15(b). It is evident that the average bulk velocity is high in the case of low slag thickness, especially in the air free space due to underdeveloped impact of the air as a result of high tuyere tip to bath surface distance.

This phenomenon can be further illustrated by comparing the average bulk velocity in the converter for all four models. Figure 16 illustrates the average matte bulk velocity profiles for lateral and combined blowing. Through observation one could infer that there is an increase in matte velocity with increased slag height, thus indicating the critical aspect of lance height for combined blowing. This is in contrast to low slag height models, which show almost equal matte velocities due to the ineffectiveness of jet penetration at a high lance height.

Implications for combined top and lateral blowing on industrial-scale converters

PSC conversion is a batch operation and meticulous control of slag and matte volumes is currently not possible. However, in previous studies (Han et al., 2001) it has been observed that high slag volumes dissipate substantial amounts of energy that would otherwise be used for recirculation and improved bath mixing. From this study, it is quite evident that there is an incentive for combined blowing as it provides energy that improves recirculation of the liquid bath. The bath to lance tip height, which affects the amount of impact energy to the bath as previous reported by Marcuson et al. (1993), is critical to the operation of combined blowing.

Conclusions

In this study, the influence of a simulated slag layer on mixing and phase dispersion characteristics and behaviour in an industrial Peirce-Smith converter (PSC) was studied experimentally, using a 0.2-scale water model, and numerically by means of 2D and 3D simulations. The results from numerical simulation with volume of fluid (VOF) and realizable turbulence model were found to be in good agreement with the experimental results. The experimental and numerical analysis results of phase distribution were in fair agreement. There appears to be a critical simulated slag
Modelling of fluid flow phenomena in Peirce-Smith copper converters

Solid-liquid mass transfer phenomena were also investigated experimentally using the cold model with the objective of spatial mapping the converter regions. The flow pattern in PSCs was found to be stratified, with high bath velocities near the bath surface. Both air flow rate and slag quantities affect dissolution behaviour in slag-matte systems. The solid-liquid mass transfer rates can be effectively controlled by close monitoring of slag quantities and air flow rates. Dead zones associated with poor dissolution rates were observed close to the sidewalls of the converter.

As a potential process alternative to prevent metal/matte losses due to splashing and wave motion in the converters, and hence to increase process efficiency, we studied combined blowing configuration in an industrial PSC with a top lance and lateral nozzles by using the 3D numerical simulations. The results revealed that wave formation and splashing can be reduced by employing combined blowing. Qualitative analysis of density contour plots suggests that combined blowing will most likely result in increased process efficiency as the energy of the top-lance injected air is utilized in reacting with new surfaces and increasing the static pressure in the system, thereby decreasing the amplitude of standing waves and thus increasing mixing efficiency, and hence the process efficiency, in the bulk liquid bath. The study also clearly demonstrated that combined blowing increases turbulence in the bath, and is thus likely to increase process throughput. A quantitative comparison of the average bulk flow liquid velocity demonstrated that simulated slag layer thickness has a great effect on the bulk recirculation velocity, as it influences the utilization of energy from the top-blown lance, thus increasing mixing efficiency. The optimal position for the lance above the liquid bath is thus critical. As the bath height varies during the blowing cycle, it might be necessary to meticulously vary the lance height during the blowing cycle to maintain a critical height.

Figure 15 – (a) Turbulent kinetic energy for lateral (L) and combined (C) blowing, and (b) velocity vector plots for low slag (S1) and high slag (S2) thicknesses in combined blowing models

Figure 16 – Average matte bulk velocity for lateral and combined blowing for S1 and S2 models

thickness in the PSC model, above which increasing air flow rate results in extended mixing times due to a combination of channelling and secondary recirculation in the slag layer. Secondary recirculation results in dissipation of energy, leading to a reduction in the bulk fluid recirculation velocity and turbulence kinetic energy. An increased matte fraction in slag and matte systems increases mixing efficiencies, possibly due to high bubble retention. It has been shown that the slag layer, as well as air flow rates, has an influence on the bulk recirculation velocity and turbulence, thus affecting the mixing efficiency in the PSC. The dispersion of simulated matte in simulated slag has been found to increase with increasing air volumetric flow rate, whereas the dispersion of simulated slag in simulated matte decreases. The difference is thought to be due to the complex interaction of phases in terms of precipitation mechanisms, coagulation, and flotation, as well as fluid motion, in the converter. The experimental results were in good agreement with the numerical simulation results in the domain of the experimental set-up.
Table II

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Typical PSC</th>
<th>Model LS₁</th>
<th>Model LS₂</th>
<th>Model CS₁</th>
<th>Model CS₂</th>
</tr>
</thead>
<tbody>
<tr>
<td>Air inlet velocity (m s⁻¹)</td>
<td>136</td>
<td>136</td>
<td>136</td>
<td>136</td>
<td>136</td>
</tr>
<tr>
<td>Blowing configuration</td>
<td>Lateral</td>
<td>Lateral</td>
<td>Lateral</td>
<td>Combined</td>
<td>Combined</td>
</tr>
<tr>
<td>Slag layer thickness (mm)</td>
<td>136</td>
<td>136</td>
<td>1360</td>
<td>136</td>
<td>1360</td>
</tr>
<tr>
<td>Matte height (mm)</td>
<td>1360</td>
<td>1360</td>
<td>1496</td>
<td>272</td>
<td>272</td>
</tr>
<tr>
<td>Combined matte and slag height (mm)</td>
<td>1496</td>
<td>1496</td>
<td>1632</td>
<td>136</td>
<td>1632</td>
</tr>
<tr>
<td>Number of tuyeres</td>
<td>42</td>
<td>1</td>
<td>1</td>
<td>2</td>
<td>2</td>
</tr>
<tr>
<td>Diameter inside refractory (mm)</td>
<td>3460</td>
<td>3460</td>
<td>3460</td>
<td>3460</td>
<td>3460</td>
</tr>
<tr>
<td>Length inside refractory (mm)</td>
<td>9140</td>
<td>217</td>
<td>217</td>
<td>217</td>
<td>217</td>
</tr>
<tr>
<td>Tuyere diameter (mm)</td>
<td>41</td>
<td>41</td>
<td>41</td>
<td>41</td>
<td>41</td>
</tr>
</tbody>
</table>

Acknowledgements

The financial support received from NRF/THRIIP funding is greatly appreciated. The authors also extend their thanks to the technical staff in the Stellenbosch University Process Engineering workshop.

References


The recovery of platinum group metals from low-grade concentrates to an iron alloy using silicon carbide as reductant

by W. Malan*, G. Akdogan*, S. Bradshaw*, and G.A. Bezuidenhout†

Synopsis
The purpose of the study was to investigate the feasibility of SiC reduction of low-grade concentrates from Lonmin's Rowland and Easterns operations with respect to metal fall and PGM recovery. These concentrates are rich in SiO₂ and MgO with low concentrations of chalcopyrite and Cr₂O₃. Pd is the most abundant of the PGMs. SiC reduction of samples was conducted at 1600°C with 2.5–3.5 kg SiC per 100 kg concentrate. PGM recoveries for Easterns concentrate were better than for Rowland. More than 85% of the Ir and Pd and almost 60% of the Pt were recovered with 3.5 kg SiC per 100 kg concentrate. SEM of slag samples showed little entrainment of metallic prills compared to Rowland samples. This was attributed to the relatively higher melt viscosities of the Rowland concentrate. In order to decrease slag viscosity and to enhance PGM recovery, the FeO content of the Easterns concentrate was increased with the addition of 10 kg converter slag per 100 kg concentrate. Ir and Pd recoveries were increased to about 95%, while Pt recovery was around 70%. On the basis of these results an optimum feed ratio between Easterns and Rowland concentrates and converter slag is proposed. Carbothermic reduction of the optimum charge was also compared to SiC reduction. Carbothermic reduction yielded a marginally higher metal fall; however, the calculated gas emissions and energy requirements were higher than for SiC reduction.

Keywords
SiC reduction, PGM recovery, LG concentrates, FactSage modelling.

Introduction
South Africa is the world's leading supplier of platinum group metals (PGMs). Most of the PGMs are contained in the Merensky and UG2 reefs of the Bushveld Complex, where they are associated with nickel- and copper-bearing minerals. In Merensky ore, the major base-metal sulphide mineral is pyrrhotite, with pentlandite, chalcopyrite, pyrite, and minor amount of other sulphides also present. In UG2 (Upper Group 2) ore the major base-metal sulphide is pentlandite. Pyrrhotite is found in moderate amounts, and millerite and pyrite in minor amounts. Because of lower mining costs, platinum mining is becoming more UG2-based, and the resulting concentrates contain high levels of chrome unless blended with Merensky ore. It is therefore critical that new and improved extraction methods be developed and exploited. The methods used in the recovery of the PGMs from these ores consist of physical concentration techniques, pyrometallurgical processing, and hydrometallurgical extraction of the base metals followed by the PGMs (Jones and Kotze, 2004; Nell, 2004).

During pyrometallurgical processing, the nickel-copper concentrates from the mill-float concentration step are smelted to bring about physical and chemical changes that enable recovery of base metals, PGMs, and other valuable metals in crude form. In general, the idea is to melt the concentrate in a furnace to produce a matte, which contains all the sulphides, below a carefully maintained slag layer. This matte, which contains large amounts of iron and sulphur, is oxidized in a Peirce-Smith converter to lower the iron and sulphur levels, while at the same time increasing the PGM grade. Conventional PGM matte smelting essentially requires the presence of a certain quantity of base metal sulphides in order to collect the PGMs in a molten sulphidic phase in the smelting furnace. However, the quantity of chrome oxide in the feed materials (particularly UG2) need to be strictly controlled to avoid the build-up of high-melting chromite spinels (Jones and Kotze, 2004; Nell, 2004).

Currently, the matte-based collection process is most widely used for PGM recovery, but because PGM-containing concentrates are becoming more enriched with UG2 concentrates, it is expected to be integrated with or replaced by an alternative processes. Mintek has developed an alternative process for smelting PGM-containing oxide feed materials that contain low sulphur levels, and often high levels of chromium oxide, known as the Conroast process. The process involves the smelting of dead-roasted sulphide concentrates...
The recovery of platinum group metals from low-grade concentrates to an iron alloy

in order to generate a small amount of an iron alloy in which PGMs and base metals are collected. A slag is also produced, which contains mostly unwanted materials and very low levels of residual PGMs. The desired degree of reduction is controlled by adjusting the carbon addition. Highly reducing conditions promote high recoveries of the valuable metals to the alloy, but high iron collection dilutes the PGM grade of the alloy, which affects the PGM recoveries in the converting and refining processes (Jones and Kotze, 2004; Nell J., 2004).

In this study, low-grade (LG) concentrates from Lonmin’s Rowland and Easterns operations were smelted with SiC as reductant. The effect of process parameters such as reductant to concentrate ratio, temperature, and different reductants on metal fall, alloy composition, slag composition, and gas composition were investigated. FactSage modelling was also used to simulate the reduction process. Detailed chemical and mineralogical characterization of the feed, alloy, and slag was conducted by X-ray diffraction (XRD), X-ray fluorescence (XRF), scanning electron microscopy (SEM), and inductively coupled plasma (ICP) analysis.

The primary objectives of this study include understanding the reducing conditions to produce the minimum amount of alloy while maintaining a high as possible recovery of PGMs; quantifying the deportment of the various elements to the alloy and slag phases, and establishing the factors affecting the recovery of PGMs; and comparing the gas emissions from different reductants in terms of environmental impact. The benefits of the new process would include no constrain on the minimum quantity of base metals required in the feed material, as the PGMs are collected in an iron-based alloy; ability to integrate the relatively large quantities of the alloy product into an existing smelter complex, possibly through a converter; allowing for the possibility of hydrometallurgical refining of the alloy; chromium tolerance; efficient PGM collection; fewer sulphur emissions compared to current matte-smelting processes; and possibly an economic incentive for treating other waste materials in a similar manner.

Materials and methods

A Carbolite STF 1800 tube furnace with a programmable Carbolite controller was used for the experiments. The alumina tube was heated by five surrounding lanthanum elements. A set point of 1600°C was set on the controller and the measured temperature recorded by a thermocouple located in the furnace. The initial plan was to attach a crucible to a wire and then suspend it from the top of the furnace at the tube outlet and lower it to the marked hot spot. However, in order to facilitate the operation, the furnace was removed from its original supporting brackets and fitted onto a fork-lifter. After the adjustment, the furnace could easily be moved up and down in vertical direction. The movement was carefully controlled by a hydraulic lever or foot pedal (Figure 1). After the furnace had reached the set temperature, the MgO crucible containing the sample mixture was placed into the tube furnace. Before the sample was placed into the hot zone, high-purity argon was allowed to purge into the Al work tube at a flow rate of 5 l/min for about 20 minutes. The sample was then raised to the hot zone, and the Ar flow rate was reduced to about 600 ml/min at the start of the experiment. After a predetermined time of reduction, the furnace was raised and the sample was allowed to cool rapidly under an Ar flow rate of 5 l/min for about 10 minutes.

The screen analysis showed that $P_{80}$ values for Easterns concentrate, Rowlands concentrate, and SiC reductant were 320 μm, 180 μm, and 380 μm respectively. The chemical compositions of the LG concentrates are given in Tables I and II.

Results and discussion

**FactSage simulations**

Initial FactSage simulations were conducted prior to laboratory-scale experiments in order to establish a range of optimum conditions. Thermodynamic equilibrium results are given in 100 kg concentrate per mass of reductant.

<table>
<thead>
<tr>
<th>Constituent</th>
<th>Rowland LG concentrate (wt %)</th>
<th>Easterns LG concentrate (wt %)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Al₂O₃</td>
<td>5.41</td>
<td>5.00</td>
</tr>
<tr>
<td>CaO</td>
<td>2.72</td>
<td>3.03</td>
</tr>
<tr>
<td>Cr₂O₃</td>
<td>2.94</td>
<td>4.31</td>
</tr>
<tr>
<td>Fe₂O₃ *</td>
<td>12.73</td>
<td>14.24</td>
</tr>
<tr>
<td>K₂O</td>
<td>0.10</td>
<td>0.10</td>
</tr>
<tr>
<td>MgO</td>
<td>22.79</td>
<td>23.05</td>
</tr>
<tr>
<td>MnO</td>
<td>0.15</td>
<td>0.18</td>
</tr>
<tr>
<td>Na₂O</td>
<td>0.38</td>
<td>0.30</td>
</tr>
<tr>
<td>P₂O₅</td>
<td>0.02</td>
<td>0.02</td>
</tr>
<tr>
<td>SiO₂</td>
<td>49.40</td>
<td>47.81</td>
</tr>
<tr>
<td>TiO₂</td>
<td>0.31</td>
<td>0.32</td>
</tr>
<tr>
<td>LOI *</td>
<td>3.08</td>
<td>2.32</td>
</tr>
<tr>
<td>Total</td>
<td>100.05</td>
<td>100.66</td>
</tr>
</tbody>
</table>

* LOI includes the total volatiles content of the rock (including the water combined in the lattice of silicate minerals) and the gain on ignition related to the oxidation of the rock (mostly due to Fe), Fe₂O₃ converted to FeO.

Figure 1 – A Carbolite STF 1800 tube furnace with controller after being modified with a fork-lifter. (1) Fork-lift, (2) argon gas inlet, (3) gas outlet with extraction fan, (4) temperature controller.

Table I

XRF results for Rowland and Easterns LG concentrates
A stoichiometric amount of SiC required per 100 kg of LG concentrate is 0.27 kg for Rowland and 0.38 kg for Easterns. These were determined as the minimum amounts of SiC required to produce a molten metal phase, primarily being Fe (> 98%), given the starting oxide concentration and ease of reduction. Experimental results are then compared with FactSage results and discussed. Without any reductant in the system, MgCr₂O₄(s) spinel accumulates, therefore a reductant mass of 3 kg SiC per 100 kg LG concentrate was chosen as a base case. During the prediction of optimum temperature range, the requirement was that Fe concentrations should be high, while Cr and Si should remain low. The respective liquidus temperatures during SiC reduction are 1420°C for Rowland and 1410°C for Easterns concentrate. The results indicated that Fe and Cr concentrations in the alloy should not be significantly affected when the temperature increased from 1400°C to 1650°C, while Si concentrations would increase. The solubility of C in the alloy decreases with increasing temperature. The metal fall is not significantly affected, however, and about 1600°C should yield a good metal fall and avoid formation of solid phases like Mg₂SiO₄(s) proto-enstatite. Therefore 1600°C was selected as the temperature at which to investigate the SiC reduction of the LG concentrates.

The effect of reductant to concentrate ratio was investigated from 0.5 kg to 4 kg SiC per 100 kg LG concentrate. It was found that an increase in reductant mass will cause more oxides, particularly FeO, to reduce, thereby increasing metal fall. For both concentrates a molten metal phase starts to form when 0.5 kg of reductant is present per 100 kg concentrate, emphasizing the ease of reduction of both concentrates, and almost all Cr₂O₃ is reduced to CrO, thereby increasing the solubility of Cr in the slag phase. The metal fall continues to rise and it therefore becomes easier to recover PGMs. Better metal fall for reductive smelting of Easterns LG concentrate is expected at higher reductant to concentrate ratios, due to the marginally higher FeO concentration. The molten metal phase consists primarily of Fe and other easily reduced base metals; however, some Cr and Si deport to the metal phase once the SiC to concentrate ratio is increased. Si and Cr start to dissolve in the molten metal at significant concentrations when the reductant mass exceeds 3 kg SiC per 100 kg LG concentrate. C concentrations in the alloy also become more significant at a higher SiC to concentrate ratio. Cr solubility in the slag phase is greatly affected by the oxidation state of Cr (Nell, 2004; Jones, 2009). Chrome in its trivalent state (spinel) has a very low solubility in the slag phase – divalent chrome, in contrast, is highly miscible in the slag phase (Nell, 2004). The FactSage simulation in Figure 2 shows how Cr is reduced from Cr(III) to Cr(II) as function of SiC additions to Easterns LG concentrate charge.

![Figure 2 – The distribution of chromium between the phases as a function of SiC additions to Easterns LG concentrate](image-url)
The recovery of platinum group metals from low-grade concentrates to an iron alloy

Experimental results

An alloy from each experiment was separated from the slag phase and weighed. The percentage metal fall for each experiment was determined as the amount of alloy formed per amount of initial concentrate. The results showed that metal fall was increased by a longer residence time (from 60 minutes to 180 minutes) and greater reductant to concentrate ratio. Some thermogravimetric analysis (TGA) experiments were also conducted to investigate the reaction mechanisms and kinetics. The alumina pedestal with the attached crucible containing the LG concentrate charge and SiC reductant were placed on a scale, which was connected to a computer with a VGA cable to acquire the change in mass of the concentrate charge. It was found that the mass of the crucible, refractory support material, and alumina pedestal remained constant throughout the experiment. Therefore the only change in mass was that of the concentrate and reductant charge in a gas-tight furnace. The mass changes on the scale were noted every 0.5 seconds on the computer, and typical graphs of mass vs time were constructed. The results showed that no significant mass changes occurred after about 10 minutes of reduction time, indicating that equilibrium was reached. The mass loss vs time were constructed. The results showed that no significant mass changes occurred after about 10 minutes of reduction time, indicating that equilibrium was reached due to the reduction of iron oxides, given their relatively high ratio. Some thermogravimetric analysis (TGA) experiments were also conducted to investigate the reaction mechanisms and kinetics. The alumina pedestal with the attached crucible containing the LG concentrate charge and SiC reductant were placed on a scale, which was connected to a computer with a VGA cable to acquire the change in mass of the concentrate charge. It was found that the mass of the crucible, refractory support material, and alumina pedestal remained constant throughout the experiment. Therefore the only change in mass was that of the concentrate and reductant charge in a gas-tight furnace. The mass changes on the scale were noted every 0.5 seconds on the computer, and typical graphs of mass loss vs time were constructed. The results showed that no significant mass changes occurred after about 10 minutes of reduction time, indicating that equilibrium was reached due to the reduction of iron oxides, given their relatively high.

\[ \text{FeO} + \text{SiC} \rightarrow \text{Fe} + \text{SiO}_2 - \text{CO} \] \[ \text{[1]} \]

Andrews (2008) also concluded that a longer residence time will improve the kinetics of matte droplet settling. Furthermore, increasing the amount of SiC causes more FeO to be reduced to Fe, causing more metal prills to form and increasing the probability of coalescence. This, once again, agrees well with previous work (Shahrokhi and Shaw, 2000; Saffman and Turner, 1956; Ammann et al., 1979). The chemical compositions of the alloys obtained from SiC reduction of Rowland and Easterns LG concentrate are shown in Tables III and IV respectively.

Fe forms the bulk of the overall composition of all of the alloys from SiC reduction of Rowland LG concentrate. This correspond well with work done by Perry et al. (1988) and Qayyam et al. (1976), who also concluded that reduction of FeO will take place before the reduction of CrO. Cr concentrations increase sharply when the reductant to concentrate ratio is increased. When the reductant to concentrate ratio is 3.5 kg SiC per 100 kg Rowland LG concentrate, Cr constitutes almost 10% in the alloy. Cr concentrations are more than 5% in alloys from tests with different reduction times. These high concentrations of Cr could cause difficulties during downstream processing, particularly during converting and in the base metals and precious metals refineries. Ni and S concentrations seem to increase with residence time. These two elements most likely originate from the mineral pentlandite. Pt and Pd concentrations remain very low in all of the alloys.

Easterns LG concentrate has a higher FeO content than Rowland LG concentrate, which explains the higher Fe content of alloys from tests with different reduction times. These high concentrations of Cr could cause difficulties during downstream processing, particularly during converting and in the base metals and precious metals refineries. Ni and S concentrations seem to increase with residence time. These two elements most likely originate from the mineral pentlandite. Pt and Pd concentrations remain very low in all of the alloys.

Easterns LG concentrate has a higher FeO content than Rowland LG concentrate, which explains the higher Fe content of alloys from tests with different reduction times. These high concentrations of Cr could cause difficulties during downstream processing, particularly during converting and in the base metals and precious metals refineries. Ni and S concentrations seem to increase with residence time. These two elements most likely originate from the mineral pentlandite. Pt and Pd concentrations remain very low in all of the alloys.

Table III

<table>
<thead>
<tr>
<th>SiC Concentrate ratio(x10^2)</th>
<th>Reduction time (min)</th>
<th>Fe</th>
<th>Cr</th>
<th>Si</th>
<th>Cu</th>
<th>Ni</th>
<th>S</th>
<th>Ir</th>
<th>Pt</th>
<th>Pd</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.5</td>
<td>60</td>
<td>81.2</td>
<td>0.24</td>
<td>&lt;0.01</td>
<td>3.67</td>
<td>&lt;0.01</td>
<td>&lt;0.01</td>
<td>0.05</td>
<td>0.02</td>
<td>0.08</td>
</tr>
<tr>
<td>3.0</td>
<td>30</td>
<td>67.6</td>
<td>8.81</td>
<td>&lt;0.01</td>
<td>2.65</td>
<td>&lt;0.01</td>
<td>&lt;0.01</td>
<td>0.04</td>
<td>0.01</td>
<td>0.08</td>
</tr>
<tr>
<td>3.0</td>
<td>45</td>
<td>71.7</td>
<td>9.36</td>
<td>&lt;0.01</td>
<td>2.36</td>
<td>&lt;0.01</td>
<td>&lt;0.01</td>
<td>0.08</td>
<td>0.01</td>
<td>0.06</td>
</tr>
<tr>
<td>3.0</td>
<td>60</td>
<td>81.4</td>
<td>2.72</td>
<td>&lt;0.01</td>
<td>2.08</td>
<td>&lt;0.01</td>
<td>&lt;0.01</td>
<td>0.05</td>
<td>0.01</td>
<td>0.04</td>
</tr>
<tr>
<td>3.0</td>
<td>75</td>
<td>76.4</td>
<td>5.9</td>
<td>&lt;0.01</td>
<td>2.25</td>
<td>&lt;0.01</td>
<td>&lt;0.01</td>
<td>0.05</td>
<td>0.01</td>
<td>0.06</td>
</tr>
<tr>
<td>3.0</td>
<td>90</td>
<td>75.1</td>
<td>6.12</td>
<td>&lt;0.01</td>
<td>2.67</td>
<td>4.42</td>
<td>1.11</td>
<td>0.04</td>
<td>0.07</td>
<td>0.04</td>
</tr>
<tr>
<td>3.0</td>
<td>180</td>
<td>74.9</td>
<td>6.35</td>
<td>&lt;0.01</td>
<td>2.71</td>
<td>4.51</td>
<td>1.13</td>
<td>0.05</td>
<td>0.08</td>
<td>0.06</td>
</tr>
<tr>
<td>3.5</td>
<td>60</td>
<td>65.1</td>
<td>9.59</td>
<td>0.01</td>
<td>2.02</td>
<td>&lt;0.01</td>
<td>0.01</td>
<td>0.04</td>
<td>&lt;0.01</td>
<td>0.05</td>
</tr>
</tbody>
</table>

Table IV

<table>
<thead>
<tr>
<th>SiC Concentrate ratio(x10^2)</th>
<th>Reduction time (min)</th>
<th>Fe</th>
<th>Cr</th>
<th>Si</th>
<th>Cu</th>
<th>Ni</th>
<th>S</th>
<th>Ir</th>
<th>Pt</th>
<th>Pd</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.5</td>
<td>180</td>
<td>81.2</td>
<td>0.24</td>
<td>&lt;0.01</td>
<td>3.67</td>
<td>&lt;0.01</td>
<td>&lt;0.01</td>
<td>0.34</td>
<td>0.02</td>
<td>0.08</td>
</tr>
<tr>
<td>3.0</td>
<td>180</td>
<td>84.5</td>
<td>1.47</td>
<td>&lt;0.01</td>
<td>1.47</td>
<td>4.49</td>
<td>2.04</td>
<td>0.8</td>
<td>0.32</td>
<td>1.24</td>
</tr>
<tr>
<td>3.5</td>
<td>180</td>
<td>88.6</td>
<td>1.33</td>
<td>0.15</td>
<td>1.08</td>
<td>2.81</td>
<td>1.52</td>
<td>0.8</td>
<td>0.65</td>
<td>1.26</td>
</tr>
</tbody>
</table>
The recovery of platinum group metals from low-grade concentrates to an iron alloy

The alloy are very favourable for downstream processing because of the difficulties in removing these elements during converting and refining. The Pt and Pd concentrations are higher in alloys from SiC reduction of Easterns LG concentrate. The better metal fall is the most likely factor to have contributed to the higher PGM concentrations in these alloys. PGM recoveries (Ir, Pd, and Pt) to the alloy phase for the respective concentrates are shown in Table V and Table VI.

From Table V it is seen that the recoveries of Ir, Pt, and Pd are very low. The highest Pt and Pd recoveries were achieved at a reductant to concentrate ratio of 5 kg SiC per 100 kg Rowland LG concentrate and residence time of 180 minutes. One factor that may contribute significantly to the low PGM recoveries is slag viscosity. The recoveries of Ir, Pd, and Pt from SiC reduction of Easterns LG concentrate are significantly better (Table VI). Ir, Pd, and Pt recoveries increase significantly when the quantity of reductant is increased. Overall, Ir has the highest recovery, followed by Pd and Pt. The very low Cr and Si concentrations in these alloys will allow for a further increase in reductant quantity and therefore it should be possible to recover more than 90% of PGMs by SiC reduction of Easterns LG concentrate.

The slag compositions from the SiC reduction of Rowland and Easterns LG concentrates are shown in Tables VII and VIII respectively.

The results from Tables VII and VIII show a significant decrease in FeO concentration compared with the initial concentrates. The lowest FeO content corresponded to the experiments with the highest quantity of reductant. The composition of the slag has a major effect on the viscosity.

### Table V

Recovery of Ir, Pd, and Pt from SiC reduction of Rowland LG concentrate

<table>
<thead>
<tr>
<th>SiC Concentrate ratio (x102)</th>
<th>Reduction time (min)</th>
<th>Ir recovery (%)</th>
<th>Pd recovery (%)</th>
<th>Pt recovery (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.5</td>
<td>60</td>
<td>2.410</td>
<td>2.198</td>
<td>0.931</td>
</tr>
<tr>
<td>3.0</td>
<td>75</td>
<td>4.449</td>
<td>3.233</td>
<td>0.86</td>
</tr>
<tr>
<td>3.0</td>
<td>90</td>
<td>3.957</td>
<td>2.637</td>
<td>6.69</td>
</tr>
<tr>
<td>3.0</td>
<td>180</td>
<td>3.816</td>
<td>3.516</td>
<td>7.514</td>
</tr>
<tr>
<td>3.5</td>
<td>60</td>
<td>4.082</td>
<td>2.905</td>
<td>0.989</td>
</tr>
</tbody>
</table>

### Table VI

Recovery % of Ir, Pd, and Pt from SiC reduction of Easterns LG concentrate

<table>
<thead>
<tr>
<th>SiC Concentrate ratio (x102)</th>
<th>Reduction time (min)</th>
<th>Ir recovery (%)</th>
<th>Pd recovery (%)</th>
<th>Pt recovery (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.5</td>
<td>180</td>
<td>11.232</td>
<td>1.538</td>
<td>0.509</td>
</tr>
<tr>
<td>3.0</td>
<td>180</td>
<td>69.728</td>
<td>62.882</td>
<td>34.95</td>
</tr>
<tr>
<td>3.5</td>
<td>180</td>
<td>94.536</td>
<td>86.629</td>
<td>59.227</td>
</tr>
</tbody>
</table>

### Table VII

Slag composition (by XRF) from SiC reduction of Rowland LG concentrate

<table>
<thead>
<tr>
<th>SiC Concentrate ratio (x102)</th>
<th>Reduction time (min)</th>
<th>Al₂O₃</th>
<th>CaO</th>
<th>CrO⁺</th>
<th>FeO⁺</th>
<th>MgO</th>
<th>SiO₂</th>
<th>TiO₂</th>
<th>Total</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.5</td>
<td>60</td>
<td>5.2</td>
<td>2.67</td>
<td>2.25</td>
<td>5.87</td>
<td>27.60</td>
<td>52.17</td>
<td>0.33</td>
<td>97.54</td>
</tr>
<tr>
<td>3.0</td>
<td>75</td>
<td>5.22</td>
<td>2.72</td>
<td>2.43</td>
<td>3.30</td>
<td>28.35</td>
<td>52.17</td>
<td>0.32</td>
<td>96.72</td>
</tr>
<tr>
<td>3.0</td>
<td>90</td>
<td>5.23</td>
<td>2.70</td>
<td>2.34</td>
<td>3.07</td>
<td>28.21</td>
<td>52.11</td>
<td>0.33</td>
<td>97.12</td>
</tr>
<tr>
<td>3.0</td>
<td>180</td>
<td>5.22</td>
<td>2.69</td>
<td>2.32</td>
<td>3.03</td>
<td>28.11</td>
<td>52.09</td>
<td>0.33</td>
<td>96.91</td>
</tr>
<tr>
<td>3.5</td>
<td>60</td>
<td>5.22</td>
<td>2.69</td>
<td>1.61</td>
<td>2.97</td>
<td>28.74</td>
<td>54.01</td>
<td>0.33</td>
<td>97.72</td>
</tr>
</tbody>
</table>

### Table VIII

Slag composition (by XRF) from SiC reduction of Easterns LG concentrate

<table>
<thead>
<tr>
<th>SiC Concentrate ratio (x102)</th>
<th>Reduction time (min)</th>
<th>Al₂O₃</th>
<th>CaO</th>
<th>CrO⁺</th>
<th>FeO⁺</th>
<th>MgO</th>
<th>SiO₂</th>
<th>TiO₂</th>
<th>Total</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.5</td>
<td>180</td>
<td>4.75</td>
<td>3.08</td>
<td>3.11</td>
<td>6.51</td>
<td>29.11</td>
<td>50.17</td>
<td>0.33</td>
<td>97.61</td>
</tr>
<tr>
<td>3.0</td>
<td>180</td>
<td>4.71</td>
<td>3.1</td>
<td>3.09</td>
<td>5.84</td>
<td>30.06</td>
<td>49</td>
<td>0.33</td>
<td>97.61</td>
</tr>
<tr>
<td>3.5</td>
<td>180</td>
<td>4.78</td>
<td>3.12</td>
<td>3.15</td>
<td>3.12</td>
<td>29.78</td>
<td>51.65</td>
<td>0.33</td>
<td>97.10</td>
</tr>
</tbody>
</table>
and FeO, NiO, CuO, and CrO will all aid in lowering the viscosity. Once the SiC comes in contact with these oxides, it will reduce and settle to join the alloy phase, thereby removing them from the slag phase and increasing the viscosity. It can be seen that the reduction process lowered the FeO concentration compared with the initial concentrate (refer to Table I).

The viscosity module in FactSage was used to determine the viscosities at 1600°C. At a temperature of 1600°C it can be safely assumed that the slag is molten. The calculated viscosities of the slags from SiC reduction of Rowland and Easterns LG concentrate at the beginning of the melts are 3.74 and 3.06 poise, respectively. The significantly higher slag viscosity for Rowland LG concentrate would make it more difficult for small metal prills to settle and coalesce.

Table IX shows viscosities of the slags at the end of the melt. The viscosities were calculated in the FactSage viscosity module from the slag compositions in Table VII and Table VIII.

Table IX shows that the calculated viscosities of the slags from all the tests are higher than the calculated viscosities at the beginning of the melts. This is because the bulk of the Fe has partitioned into the alloy. Some Cr has also deported to the alloy phase. The viscosities of slags from SiC reduction of Rowland LG concentrate are significantly higher than slags from SiC reduction of Easterns LG concentrate. This could explain why the PGM recoveries from Rowland LG concentrate are significantly lower.

Viscosities of PGM smelting slags are reported in the literature (Eric, 2004; Eric and Hejja, 1995) as being in the range 1.5–4 poise, which could hinder the settling of particles 15 μm or smaller in size. The FeO/SiO₂ ratio of the slag seems to have a major influence on the viscosity. The Rowland LG concentrate under investigation has a lower FeO/SiO₂ ratio than Easterns LG concentrate. When FeO is reduced, slag viscosity will increase and valuable metal prills will not settle. The high initial slag viscosity will contribute to insufficient coalescence of metal prills and phase separation. The corresponding viscosities from these experiments conducted with Rowland LG concentrate fall mostly above the range of 1.5–4 poise. It therefore seems that high slag viscosities are the primary reason for the low PGM recoveries. Slag viscosities from SiC reduction of Easterns LG concentrate do, however, fall in the recommended range. The lower viscosities will aid in the coalescence of metal prills, enhance phase separation, and induce good PGM recovery.

Figures 3 and 4 are SEM images of the slag phases from SiC reduction of Rowland and Easterns LG concentrate.

![Figure 3 – SEM image of slag phase (darker) containing metallic prills (bright spots) from Rowland LG concentrate. Smelting time 180 min, reductant to concentrate ratio 3 kg SiC per 100 kg concentrate](image1.png)

![Figure 4 – SEM image of the slag from Eastern LG concentrate. Smelting time 180 min, reductant to concentrate ratio 3 kg SiC per 100 kg concentrate](image2.png)
respectively, from experiments that had the same reductant to concentrate ratio and reduction time.

Figure 3 shows a SEM image of the slag phase from SiC reduction of Rowland LG concentrate. Metal prills are entrained in the slag. These metal prills are very small and are most likely trapped in the slag phase and will never settle or coalesce with other metal prills of similar size. Studies in the literature indicate that many small metal prills (< 2 μm) are expected never to settle under the force of gravity alone. This phenomenon agrees well with the work done by Fagurland and Jalkanen (1999) and Poggie et al. (1969), who also reported that very small droplets may either settle very slowly or may be trapped as ‘rafts’ of droplets floating on the top surface of the slag or as droplets suspended below small gas bubbles. However, the high viscosity of the slag is most likely restricting the coalescence and settling of metal prills. An EDX spot analysis on the metal prill indicated by the arrow detected Ir and Pd.

Figure 4 shows a SEM image of the slag phase from SiC reduction of Easterns LG concentrate. The slag phase is smoother, with no metal prills entrained. This is an indication that metal prills coalesced and settled well within the slag phase. From these findings it is very clear that the lower slag viscosity contributes significantly to PGM recovery from SiC reduction of Easterns LG concentrates. This corresponds to similar findings in the literature (Shahrokhi and Shaw, 2000; Saffman and Turner, 1956; Ammann et al., 1979).

From the results obtained experimentally, it was concluded that Easterns LG concentrate should form the bulk of the dry LG concentrate feed to a DC arc furnace, since it has a higher FeO/SiO\textsubscript{2} ratio, which is significant in reducing slag viscosity and increasing overall PGM recovery. The slag viscosities need to be kept in the region of approximately 3.2 poise (average viscosity determined from experiments with SiC reduction of Easterns LG concentrate) for acceptable PGM recoveries. Rowland and Easterns concentrates could be combined, with the main fraction being Easterns, or another source added that would lower slag viscosity. The slag from a Peirce-Smith converter has a high FeO/SiO\textsubscript{2} ratio and could be used to reduce the slag viscosity. FactSage was used to model such a scenario and an experiment was also conducted to back up the results. FactSage modelling was conducted at 3.5 kg SiC per100 kg Easterns LG concentrate at 1600°C with varying amounts of converter slag additions.

Figure 5 shows that addition of converter slag does decrease the slag viscosity. The converter slag is rich in FeO and thereby the FeO/SiO\textsubscript{2} ratio in the slag is increased, causing the slag viscosity to decrease. However, the converter slag contains about 50 wt% SiO\textsubscript{2}, which could act to increase the slag viscosity. Figure 5 shows that an increase in reductant will cause more FeO to be reduced, consequently a system with 5 kg and 10 kg converter slag additions will have a higher slag viscosity than a system with no converter slag if the reductant additions are increased past the point of intersection. Another critical point is that the conductivity and viscosity of the slag are inversely related. A decrease in viscosity will increase the conductivity of the slag; increasing iron oxide serves to depolymerize the slag and creates sites for electronic conduction (Nell, 2004; Eric, 2004). It is clear from the findings that around 10 kg of converter slag addition per 100 kg concentrate would decrease slag viscosity without increasing the total quantity of slag significantly. The alloy is also expected to have a good PGM grade. A test was therefore conducted to compare the results from experiments and FactSage modelling for similar conditions.

From Table X, it is apparent that FactSage predicts a slag with similar composition. The marginally lower FeO/SiO\textsubscript{2} ratio in the slag from FactSage modelling will cause the viscosity to be somewhat higher than the slag from the experiment. Table X also shows an improved PGM recovery with converter slag addition, which is likely to be a result of the decrease in slag viscosity. The Pd and Ir recoveries are nearly 100%, compared to Pd and Ir recoveries of 94.5 and 86.6% obtained experimentally with no slag addition. Pt recovery has also improved, from 59.2% to almost 70%. Pt recovery is expected to improve if the metal fall increases. More reductant could be added to increase metal fall and thereby increase the Pt recovery from the initial concentrate. Overall, this is this is a significant finding. A portion of converter slag can therefore be recycled and re-melted.
The recovery of platinum group metals from low-grade concentrates to an iron alloy

together with any LG concentrate to increase metal fall and PGM recoveries.

FactSage modelling was used to predict an optimum ratio between Rowland and Easterns LG concentrates. The reductant to concentrate ratio was fixed at 3.5 kg SiC per 100 kg LG concentrate and the temperature at 1600°C. FactSage predicted that adding more than 30 kg converter slag per 100 kg LG concentrate decreases the alloy to slag ratio. Therefore a 0.7–0.8 fraction of Easterns LG concentrate in the feed and 20–30 kg converter slag per 100 kg LG concentrate should not significantly increase furnace slag quantities and the FeO/SiO\textsubscript{2} ratio should be adequate to sustain a slag viscosity close to 3.5 poise. At these operating conditions more than 90% of the PGMs should be recovered from a LG concentrate feed in an alloy with a high PGM grade. Cr and Si concentrations in the alloy are less than 1% in total, and C concentrations are less than 1%.

FactSage modelling was also undertaken to compare SiC reduction with carbon reduction. The optimum feed conditions, namely 75% Easterns LG concentrate, 25% Rowland LG concentrate, 25 kg converter slag per 100 kg LG concentrate, and 0–4 kg reductant per 100 kg LG concentrate at 1600°C were used in the comparison. With these conditions, it is assumed that slag viscosity will be low enough to ensure good phase separation and PGM recovery. The results indicated that C reduction of a LG concentrate charge results in a marginally higher metal fall. The alloy compositions were very similar and only small differences in Fe, Cr, and Si concentrations were noted. Gas emissions and energy requirements are higher for C reduction, arguably due to C reacting endothermically with FeO to produce Fe(l) and CO(g) in contrast to SiC reacting exothermically with FeO to produce Fe(l), SiO\textsubscript{2}(l) and CO(g).

However, it must be borne in mind that SiC is not a naturally occurring compound and is manufactured by carbothermic reduction of silica at high temperatures, which entails its own high level of emissions which should be added to the emissions from SiC smelting. A preliminary FactSage analysis was conducted for the reaction to produce SiC:

$$\text{SiO}_2(s) + 3\text{C}(s) \rightarrow \text{SiC}(s) + 2\text{CO}(g) (+ \text{O}_2 \rightarrow 2\text{CO}_2) \ [3]$$

The resulting estimates of energy requirements and CO emissions per ton of SiC product are given in Table XI. It is seen from Table XI that not all of the SiO\textsubscript{2} and C has

\begin{table}
\centering
\textbf{Table X}
\caption{Effect of adding converter slag – comparison between experimental results and FactSage modelling}
\begin{tabular}{|c|c|c|}
\hline
& Experimental with slag & FactSage modelling with slag \\
\hline
\textbf{Metal fall %} & 8.82 & 10.5 \\
\hline
\textbf{Alloy} & \textbf{wt %} & \textbf{wt %} \\
\hline
Fe & 85.3 & Fe & 95.687 \\
Cr & 4.13 & Cr & 1.172 \\
Si & 2.73 & Si & 0.0565 \\
Cu & 1.10 & Cu & 0.982 \\
Ni & 2.59 & Ni & 1.95 \\
S & 1.53 & S & Not included in feed \\
Ir & 0.81 & Ir & Not included in feed \\
Pd & 1.21 & Pd & Not included in feed \\
Pt & 0.65 & Pt & Not included in feed \\
\hline
\textbf{Slag} & \textbf{wt %} & \textbf{Slag} & \textbf{wt %} \\
\hline
Al\textsubscript{2}O\textsubscript{3} & 4.4 & Al\textsubscript{2}O\textsubscript{3} & 5.358 \\
CaO & 2.95 & CaO & 3.154 \\
CrO & 3.88 & CrO & 3.691 \\
FeO & 7.657 & FeO & 6.809 \\
MgO & 28.85 & MgO & 23.997 \\
SiO\textsubscript{2} & 49.75 & SiO\textsubscript{2} & 56.588 \\
TiO\textsubscript{2} & 0.32 & TiO\textsubscript{2} & Not included in feed \\
\hline
\textbf{Alloy} & \textbf{Recovery %} & \textbf{Alloy} & \textbf{Recovery %} \\
\hline
Ir & 97.867 & Ir & 100 % \\
Pd & 97.040 & Pd & 100 % \\
Pt & 69.086 & Pt & 100 % \\
\hline
\end{tabular}
\end{table}

\begin{table}
\centering
\textbf{Table XI}
\caption{Thermodynamic analysis of stoichiometric feed of SiO\textsubscript{2} and C to produce 1 ton of SiC}
\begin{tabular}{|c|c|c|c|}
\hline
\textbf{Temperature (°C)} & \textbf{SiC product produced (kg)} & \textbf{CO emissions (kg)} & \textbf{ΔH – energy required (MJ)} \\
\hline
1600 & 987.6 & 1388.19 & 19837.95 \\
1800 & 979.9 & 1382.94 & 20481.99 \\
2000 & 969.9 & 1376.23 & 21138.51 \\
2200 & 954.8 & 1368.26 & 21843.21 \\
2500 & 834.9 & 1334.35 & 24040.73 \\
\hline
\end{tabular}
\end{table}
The recovery of platinum group metals from low-grade concentrates to an iron alloy

reacted to form SiC. Thermodynamic modelling predicts that a small fraction of the SiO$_2$ will be converted to SiO(g), leaving some unreacted C(s) in the system. Overall more than 1.3 t of CO (g) is emitted to produce 1 t of SiC. Moreover, the energy required to produce the given SiC quantities will contribute to overall energy requirements for recovery of PGMs from an iron alloy. This needs to be taken into consideration from an environmental and economic point of view when considering a reductive smelting route. It was, however, determined that only approximately 35 kg SiC per ton of LG concentrate is required to recover most of the PGMs. It must also be taken into consideration that these PGMs need to be extracted from a more enriched LG concentrate feed, and reductive smelting is the only feasible option at the present time.

Conclusions
The feasibility of using SiC as reductant for Rowland and Easterns LG concentrates was investigated with respect to metal fall, PGM grade in the alloy, slag composition, and PGM recovery, using small-scale experiments in combination with FactSage modelling. The findings can be summarized as follows.

- SiC reduction of Easterns LG concentrate resulted in significantly better metal fall and PGM recoveries compared with Rowland concentrates. At a reductant to concentrate ratio of 3.5 kg SiC per 100 kg Easterns LG concentrate, more than 85% of Ir and Pd were recovered, and more than 60% of Pt. The higher FeO/SiO$_2$ ratio of Easterns LG concentrate and consequent lower slag viscosity is most likely to have contributed to the improvement of recoveries. SEM images from a slag from SiC reduction of Easterns LG concentrate showed no entrained metal prills, indicating that most metal prills had coalesced and settled. Cr and Si concentrations were below 2% in total in all alloys.

- In order to improve the PGM recoveries, the FeO content of the initial charge had to be increased. Peirce-Smith converter slag from Lonmin was used as an addition to increase FeO/SiO$_2$ ratio. The experiments resulted in more than 95% recoveries for Ir and Pd, together with about 70% for Pt. FactSage modelling predicted that Easterns LG concentrate should make up 70–80% of the LG concentrate charge and 20–30 kg converter slag be added per 100 kg LG concentrate to attain relatively lower viscosities for phase separation. It is expected that PGM recoveries of more than 90% should be obtained from the LG concentrate, in conjunction with a good PGM grade in the alloy.

- Using the optimum LG concentrate charge, the effectiveness of SiC as a reductant was also compared to that of C through thermodynamic modelling. C reduction of a LG concentrate charge led to a marginally higher metal fall at the same reductant to concentrate ratio compared with SiC reduction. The alloy composition was very similar and only small differences in Fe, Cr, and Si concentrations were noted. Gas emissions and energy requirements were higher for C reduction of a LG concentrate charge.

- From the evidence, it is clear that SiC reduction seems a reasonably attractive alternative to carbon-based reductants. Therefore, integrating this process into the present matte-based collection flow sheet could be considered as a future alternative for smelting LG concentrates. However, it must be borne in mind that SiC is not a natural compound and it should be manufactured by again carbothermic reduction of silica at high temperatures with its own level of emissions. This obviously will require further investigation.

Acknowledgements
The authors wish to thank Lonmin Plc for the financing of this work.

References


Solid advantage

RCS® technology maximizes flotation performance

Proven at more than 600 installations worldwide, Metso's RCS® flotation technology combines a circular tank design with our patented DV™ deep-vane impeller. The result is a powerful radial flow and slurry recirculation that maximizes flotation performance for all roughing, cleaning and scavenging duties. With improved performance, simplified maintenance and reduced operating costs, you can rely on Metso’s equipment and service. They’re both rock solid.

BEE Ownership Compliant

metso.com – email: mmsa.info.za@metso.com
Value-in-use model for chlorination of titania feedstocks

by S. Maharajh*, J. Muller*, and J.H. Zietsman†

Synopsis
In the chlorination process for TiO₂ pigment production, blends of titania feedstocks such as ilmenite, synthetic rutile (SR), natural rutile, upgraded slag, and chloride-grade slag are reacted with coke and chlorine at a temperature of around 1000°C to form TiCl₄ (the main product) and other waste metal chlorides. The TiCl₄ is the main feed material for the TiO₂ pigment-making process. Feeding different titania materials to the chlorinator affects the amount of coke and chlorine required for the process, the amount of waste generated, waste disposal costs, the amount of TiCl₄ produced, and bed build-up rates. These factors influence the value of the feedstock. Generally, a higher TiO₂ feedstock is more valued since less waste is generated and less reagents are consumed. To quantify the impact of different feedstocks on the chlorinator, a techno-economic model was developed to describe the chlorination process and estimate process variables at steady state. This paper describes the development of the model and studies in which the model has been used to quantify effects of using different feedstocks.

Keywords
titania feedstock, chlorination, process modelling TiCl₄, value-in-use.

Introduction
Approximately 90% of all TiO₂ extracted from titanium-bearing minerals is used to produce white pigment (TZMI, 2012). A significant portion of this pigment is produced through the chloride process. This involves chlorination of TiO₂ feedstocks such as natural and synthetic rutile, ilmenite, and high-titania slag in a fluidized-bed reactor to produce TiCl₄, which is subsequently purified and oxidized to produce TiO₂. The chloride process has stringent feedstock quality specifications to ensure that it can be operated in a stable and economical manner.

As a major TiO₂ feedstock producer, Exxaro Heavy Minerals (now part of Tronox) needed to gain a thorough understanding of how their products would behave in their customers’ chlorination reactors. This understanding would firstly assist in ensuring that an acceptable product is produced. Secondly, it would make it possible to gauge the value of the products in the hands of customers. To improve this understanding, it was decided to develop a techno-economic model of the chloride process that could be used to study the influence of different feedstock characteristics on the performance of the pigment production process.

Process analysis
This section presents details of the process analysis done with the purpose of collecting information that could be used as the basis of the modelling work.

Process description
The purpose of the chloride TiO₂ pigment production process is to extract the maximum amount of titanium from the TiO₂-containing feed material in the form of titanium dioxide, while rejecting as much of the impurities (e.g. Ca, Mg, Si, Al, etc.) as possible to the waste streams, based on differences in the phase transition temperatures of different metal chlorides (Table I). An overview of the process is shown in Figure 1. The process consists of the following five stages (Lee 1991).

➤ Chlorination. This first stage is the focus of this paper. Chlorination converts feed materials to a solid waste stream and a crude liquid stream containing most of the titanium as TiCl₄.

➤ Purification. The crude TiCl₄ produced in chlorination contains a wide range of impurities, which include solid iron and manganese chlorides, and unreacted ore, coke, and silicates, as well as soluble vanadium. Vanadium is converted to an insoluble chloride, and all the solid impurities are removed by vaporizing the TiCl₄ and condensing it again.

➤ Oxidation. Liquid TiCl₄ from purification is vaporized and reacted with pre-heated oxygen to produce TiO₂ and chlorine (Equation [1]). Chemicals are added for...
crystallization control, and the mixture of solids and gases is cooled before separation. The gas is recirculated to chlorination

\[ TiCl_4(g) + 2O_2(g) \rightarrow TiO_2(s) + Cl_2(g) \]  

➤ Surface Treatment. The TiO_2 particles are treated to improve their properties for specific pigment applications. This stage involves surface coating, washing, and de-watering to arrive at a final pigment product

➤ Dispersion and packaging. The final stage ensures that the product is in a suitable form and packaging for the intended application.

Details of the chlorination stage of the process are shown in Figure 2. The equipment consists of a continuous fluid bed chlorinator, a solids removal cyclone, a condensation unit, and a gas scrubber.

The chlorinator receives ore, coke, and chlorine as its main inputs. Some crude liquid TiCl_4 is recycled to the chlorinator as a coolant for temperature control. Some of the solids blown over in the chlorinator are recovered by the cyclone and recirculated.

The combination of the cooled off-gas duct from the chlorinator and the solids removal cyclone is referred to as the ‘cross-over and cyclone’. Recycled crude liquid TiCl_4 is used as a coolant in the cross-over section. Cooling results in some of the chlorides precipitating as solids. The cyclone separates the coarsest solids from the vapour and fine solids. The coarse particles, which are a result of blow-over, are recycled back to the chlorinator.

The condensation unit splits the inlet gas stream into crude liquid TiCl_4 and a gas stream. The gas is cleaned in the scrubber, and the crude TiCl_4 is partially recycled and the remainder fed to the purification section.


\[ TiO_2(s) + C(s) + 2Cl_2(g) \leftrightarrow TiCl_4(g) + CO_2(g) \]
\[ \Delta H_{298} = -211.9 \text{ kJ/mol TiO}_2 \]  

\[ 2MO_x(s) + xC(s) + 2xCl_2(g) \leftrightarrow 2MCl_{2x}(l/g) + xCO_2(g) \]
\[ M = Fe, Ca, Mg, Al, etc. \]
\[ \Delta H_{298} = -82.1 \text{ kJ/mol FeO} \]

\[ CO_2(g) + C(s) \leftrightarrow 2CO(g) \]
\[ \Delta H_{298} = 172.5 \text{ kJ/mol CO}_2 \]
Value-in-use model for chlorination of titania feedstocks

2H₂O(l) + C(s) + 2Cl₂(g) ⇌ 4HCl(g) + CO₂(g)  \[5\]

The chlorination reactor is operated at temperatures of around 1000°C. During chlorination most of the metal oxides are converted to chlorides and evaporated into the gas phase. High boiling-point chlorides such as CaCl₂ and MgCl₂ tend to remain in the bed as liquids, causing operational problems. SiO₂ and ZrO₂ tend not to chlorinate, and accumulate in the bed as solids. These problematic solids and liquids are bled from the bed to avoid build-up. Carbon binds to the oxygen in the metal oxides and leaves the reactor as a mixture of CO and CO₂. Moisture tends to react with chlorine and carbon to form hydrogen chloride gas. The gaseous chlorides and other gas species leave the reactor and are cooled, causing most of the impurity metal chlorides to revert to the solid state, but leaving TiCl₄ in the vapour phase (Lee, 1991).

The reactions occurring in the chlorinator are mostly exothermic. For example, when the reagents in Equation [2] are combined at 25°C adiabatically, the system would reach a temperature in excess of 1500°C. For this reason crude liquid TiCl₄ is charged into the chlorinator as a coolant for temperature control. This input stream was not included explicitly in the model, but due to the assumption of isothermal equilibrium and the fact that separation efficiency is specified and not modelled, this has a negligible effect on the model results.

Material descriptions
To operate the chlorinator efficiently, the TiO₂ feed materials have to comply with stringent quality specifications (Stanaway, 1994b).

- The bulk density and particle size distribution must support fluidization of the bed, while minimizing blow-over of unreacted particles into the gas stream. The TiO₂ feedstock particle sizes must typically be smaller than 850 μm and larger than 100 μm. The bulk density of the material must be more than 2 kg/l
- The alkali oxide content (MgO and CaO) must be very low since the alkali chlorides are liquid at chlorinator operating temperatures, and can cause clogging of the bed
- Although most of the feed materials contain some iron, the iron content must be limited to minimize iron chloride waste generation and reactant consumption, and maximize plant capacity
- Chromium and vanadium can cause toxicity of the iron chloride waste. The levels of these elements in the feed must be limited
- Feed silica content must be limited to prevent build-up in the chlorinator
- Tin and arsenic tend to remain in the TiCl₄ stream after purification, contaminating the final product. Feed materials must therefore be low in these elements
- Uranium and thorium are radioactive and concentrate in waste and product streams, causing health and safety risks. Very stringent specifications on these elements are enforced.

A typical chemical composition specification for high-TiO₂ slag is shown in Table II.

Coke is ground to a particle size suitable for fluidization before use. This material also has to be of high purity to limit the introduction of impurity oxides into the process. Industrial-grade chlorine is used in the main chloride feed stream. The recycled chlorine is less pure than the fresh chlorine.

Key phenomena
Given the purpose of the model, the most important process phenomena that had to be included were the following:

- Chemical reactions. The chemical reactions converting feed to product are the essence of the chlorination reactor. These are affected by both feedstock properties and operating conditions
- Blow-over. The entrainment of particles in the gas product stream from the chlorinator has an influence on the value of a particular feed material in the chlorination reactor
- Cyclone separation. The recovery of coarse particles in the cyclone and recycling to the chlorinator is of similar importance to blow-over.

Model development
The purpose of the model was to conduct techno-economic calculations to evaluate the influence of different feed materials and operating conditions on the behaviour and performance of the chlorination process. For this reason it was decided to employ a steady-state model based on the process mass and energy balance.

The equipment incorporated into the model included the chlorinator, the off-gas cooling duct and cyclone (cross-over and cyclone), and the condensation unit that separates the products into gas, liquid, and waste streams.

Table II

<table>
<thead>
<tr>
<th>Compound</th>
<th>Specification</th>
</tr>
</thead>
<tbody>
<tr>
<td>SiO₂</td>
<td>&lt; 2.00%</td>
</tr>
<tr>
<td>Al₂O₃</td>
<td>&lt; 1.50%</td>
</tr>
<tr>
<td>CaO</td>
<td>&lt; 1.13%</td>
</tr>
<tr>
<td>MgO</td>
<td>&lt; 1.20%</td>
</tr>
<tr>
<td>MnO</td>
<td>&lt; 2.00%</td>
</tr>
<tr>
<td>Cr₂O₃</td>
<td>&lt; 0.50%</td>
</tr>
<tr>
<td>V₂O₅</td>
<td>&lt; 0.50%</td>
</tr>
<tr>
<td>U+Th</td>
<td>&lt; 100 ppm</td>
</tr>
</tbody>
</table>
Value-in-use model for chlorination of titania feedstocks

The remaining solids and gas are combined with cooling TiCl₄ and equilibrated to generate the final product stream from this section. The product from the cross-over and cyclone is split between waste solids, a gas product, and a crude liquid TiCl₄ product.

Model variables and parameters

The material input variables supplied to the model by the user are listed in Table III, and the remaining input variables in Table IV. The model parameters are presented in Table V.

The material stream values calculated by the model are shown in Table VI. In addition to these variables, those listed in Table VII are also calculated.

Assumptions

The following assumptions were made in the model.

➤ The content of the fluid bed reactor is homogeneous in terms of temperature, particle size distribution, and chemical composition. This assumption is implicit in the lumped parameter modelling approach applied. The assumption is not true, but it does not have a detrimental influence on the modelling results, given the purpose of the model

➤ Chlorinator reactions run to equilibrium. This assumption and the next one were required to make it possible to solve the model. Very little detail was available on the actual chemical reaction behaviour of the process, since access to a plant was not possible. The model results based on this assumption were deemed to be acceptable for the purpose of the work

➤ Material reaches equilibrium in the cross-over

➤ Coke is assumed to be pure graphite. This assumption was made to simplify the model, and to focus it on the influence of the TiO₂ feedstock rather than the coke. This means that sulphur is ignored by the model. Sulphur leaves the system through the waste gas system as sulphur species such as H₂S, COS, and SOCl₂. It has a limited influence on the chlorination phenomena of interest here

➤ Liquid phases are immiscible. For simplicity, all liquid compounds were handled separately as pure substances, and not as a mixture. This reduced the driving force for liquid formation because the activities of all the liquid compounds are unity. This assumption would have introduced inaccuracies into the equilibrium calculations

➤ Particles are compositionally homogeneous

➤ Chlorine slip is usually low and therefore was assumed to be zero in the model. Chlorine slip occurs when chlorine passes through the chlorinator bed unreacted. This phenomenon reduces chlorine efficiency and indicates a chlorinator bed issue (e.g. high SiO₂ content, low carbon content).

Material definitions

The materials in the model were described with thermochemical data from the FACT pure substance database in FactSage 5.5. The compounds included in the model are listed in Table VIII.

Examples of TiO₂ feedstock assays are shown in Table IX. Coke, chlorine, oxygen, and nitrogen were all treated as pure streams. Air was entered as a 79% N₂, 21% O₂ mixture on volume basis.

Some examples of particulate material properties for synthetic rutile and slag are shown in Tables X and XI.

Physical phenomena

Chemical reactions were modelled very simply through equilibrium calculations using the ChemApp thermochemistry library (Petersen and Hack, 2007), and data from FactSage (Bale et al., 2009).

Blow-over of solids in the chlorinator and subsequent recovery of coarse solids in the cyclone were the only physical phenomena that were modelled in detail, and are described here.

In the chlorinator, solids are entrained in the fluidizing gas and elutriated out of the chlorinator unit. This mass is significant and therefore had to be included in the model. Due to the complexities and uncertainties surrounding elutriation, a simplified methodology was used based on the following model input parameters for each feedstock material:

➤ Density – the solid density of the feedstock material

➤ Particle size distribution – the particles sizes and mass fraction of each size class for each feedstock

➤ Particle size elutriation constants (Kᵢ) – the elutriation constants for each particle size class for each feedstock

➤ Particle size cyclone separation efficiency – the fraction of material of each particle size class recovered in the cyclone

➤ Composition – the composition of the feedstock material, which is assumed to be constant throughout each particle and to remain the same until it is blown out of the reactor.

In test work, the particulate solids elutriation constants are determined in units of kg/(s.m²). These constants are a function of particle shape, density, and size. This implies that for a reactor of a given area, a certain flux of solids of a specific particle size is expected in the outlet. Data on the
fluidization of TiO₂ feedstocks has been previously investigated (Moodley et al., 2012).

At steady-state operation the rate of particles blown over is limited to the incoming rate of particles of that size. For this system, the following are the sources of particles of a specific size:

➤ Feed material. Material feed is classified, and the particles of a certain average particle size enter at a specified total feed rate multiplied by the fraction of material with that average particle size

➤ Recycled blow-over feed. Using the elutriation constant for a particular particle size class, the rate at which particles are blown over is calculated, with only some of these being removed in the cross-over and cyclone section. The blow-over rate is therefore multiplied with the separation efficiency in the cyclone for a particle size class to calculate the rate at which particles of a size class are recycled

➤ Larger size particles reacting. Chemical reactions in the chlorinator cause particles to shrink and hence fall into smaller size classes. This feed rate of particles into a lower size class is determined from the average particle

\[ F_{bo,i} = MIN \left( \frac{F_{in,i}}{1.6 - X_{er,i}} \cdot K_i \cdot A \cdot 3600 \right) \]  

**Table III**

<table>
<thead>
<tr>
<th>Stream</th>
<th>Feed rate</th>
<th>Composition</th>
<th>Temperature</th>
<th>Compounds</th>
</tr>
</thead>
<tbody>
<tr>
<td>TiO₂ feed</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td>TiO₂, Ti₃O₇, Fe₂O₃, Fe₃O₇, ZrO₂, SiO₂, Cr₂O₃, Al₂O₃, P₂O₅, MnO, CaO, MgO, V₂O₅, Nb₂O₅, H₂O₂, SnO₂</td>
</tr>
<tr>
<td>Coke feeds</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td></td>
</tr>
<tr>
<td>Cl₂(g) feed</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td>Cl₂</td>
</tr>
<tr>
<td>N₂(g)</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td>N₂</td>
</tr>
<tr>
<td>O₂(g)</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td>O₂</td>
</tr>
<tr>
<td>Air</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td>N₂, O₂</td>
</tr>
<tr>
<td>Cl₂(g) recycle</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td></td>
</tr>
<tr>
<td>Recycle blow-over</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td></td>
</tr>
<tr>
<td>Chlorinator cooling TiCl₄</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td>TiCl₄</td>
</tr>
<tr>
<td>Cross-over cooling TiCl₄</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td>TiCl₄</td>
</tr>
</tbody>
</table>

**Table IV**

<table>
<thead>
<tr>
<th>Variable</th>
<th>Description</th>
<th>Typical value</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>Feedstock basis</td>
<td>Total feedstock rate used as basis for the calculations. Each feedstock’s rate is calculated using this value and the fraction of the feedstock in the mix</td>
<td>8100</td>
<td>kg/h</td>
</tr>
<tr>
<td>Operating temperature</td>
<td>Temperature at which the chlorinator is operated and the products exit from chlorinator</td>
<td>1050</td>
<td>°C</td>
</tr>
<tr>
<td>Cross-over temperature</td>
<td>Temperature at which the material exits from the cross-over unit</td>
<td>200</td>
<td>°C</td>
</tr>
<tr>
<td>Product final temperature</td>
<td>Final temperature of the solid, liquid, and gas product out of the system</td>
<td>70</td>
<td>°C</td>
</tr>
<tr>
<td>Off-gas CO:CO₂ molar ratio</td>
<td>Molar ratio of CO and CO₂ in the gas product out of the chlorinator</td>
<td>1</td>
<td></td>
</tr>
<tr>
<td>Bed inert cut-off fraction</td>
<td>Maximum percentage of inerts in the bed</td>
<td>40</td>
<td>%</td>
</tr>
<tr>
<td>Mass Ti oxides unreacted set-point</td>
<td>Amount of unreacted Ti oxides in the chlorinator reaction mixture to solve the amount of chlorine required. Should be a small value larger than 0</td>
<td>0.2</td>
<td>kg/h</td>
</tr>
<tr>
<td>Chlorinator TiCl₄ cooling percentage of product flow</td>
<td>Fraction of the chlorinator product flow rate used to calculate the rate of TiCl₄ cooling</td>
<td>0.025</td>
<td></td>
</tr>
<tr>
<td>Cross-over TiCl₄ cooling ratio of product flow</td>
<td>Ratio of TiCl₄ added to the cross-over for cooling relative to the TiCl₄ production rate in the chlorinator</td>
<td>1</td>
<td></td>
</tr>
<tr>
<td>Percentage Cl₂ recovered</td>
<td>Percentage of chlorine recovered from the circuit</td>
<td>99</td>
<td>%</td>
</tr>
<tr>
<td>Blow-over reductant solids removal efficiency</td>
<td>Fraction of the reductant solid blow-over removed from the chlorinator output stream, and recycled</td>
<td>90</td>
<td>%</td>
</tr>
<tr>
<td>Chlorine feed initial value</td>
<td>Initial value of chlorine feed for the first iteration of the model</td>
<td>13,660</td>
<td>kg/h</td>
</tr>
<tr>
<td>Reductant feed initial value</td>
<td>Initial value of reductant feed for the first iteration of the model</td>
<td>1,439</td>
<td>kg/h</td>
</tr>
<tr>
<td>Chlorine recycle initial value</td>
<td>Initial value of recycled chlorine feed for the first iteration of the model</td>
<td>0</td>
<td>kg/h</td>
</tr>
</tbody>
</table>

**Table V**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
<th>Typical value</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bed volume</td>
<td>Volume of the solids bed</td>
<td>20</td>
<td>m³</td>
</tr>
<tr>
<td>Bed area</td>
<td>Volume of the fluidized bed</td>
<td>7</td>
<td>m²</td>
</tr>
</tbody>
</table>

**Table VI**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
<th>Typical value</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>F_{bo,i}</td>
<td>Minimum of the input rate of particles and the value calculated from the elutriation constant. This approach ensures that the blow-over rate is constrained by a mass balance over the chlorinator. The variable used in the blow-over and cyclone recovery calculations are defined in Table XII.</td>
<td>[ F_{bo,i} = MIN \left( \frac{F_{in,i}}{1.6 - X_{er,i}} \cdot K_i \cdot A \cdot 3600 \right) ]</td>
<td></td>
</tr>
</tbody>
</table>
Value-in-use model for chlorination of titania feedstocks

### Table VI

**Model material output streams. Values for feed rate, composition, and enthalpy are calculated for all the streams**

<table>
<thead>
<tr>
<th>Stream</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Chlorinator output</td>
<td>Gas product from the chlorinator equipment, containing solid feed material carried over</td>
</tr>
<tr>
<td>Bleed solids</td>
<td>Solids and liquids forming in the chlorinator, which build up over time and are removed periodically as a bleed stream</td>
</tr>
<tr>
<td>Cross-over output</td>
<td>Output from the cross-over section containing cooled gas and carried-over feed solids not recovered and recycled</td>
</tr>
<tr>
<td>Gas product</td>
<td>Gas product from the chlorination circuit that includes CO, CO(_2), O(_2), etc. This stream excludes any gas species forming due to impurities in the feed materials</td>
</tr>
<tr>
<td>TiCl(_4)(aq)</td>
<td>Liquid TiCl(_4) product from the chlorination circuit</td>
</tr>
<tr>
<td>Solid/liquid/gas</td>
<td>All the solid, liquid, or gas species forming due to impurities in the feed materials that are not removed in any other stream from the chlorination circuit</td>
</tr>
</tbody>
</table>

### Table VII

**Model output variables**

<table>
<thead>
<tr>
<th>Variable</th>
<th>Description</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>Chlorinator energy requirement</td>
<td>Energy balance over the chlorinator unit. This value is calculated as the chlorinator output enthalpy, minus the cooling TiCl(_4) enthalpy and enthalpies of all feed material streams</td>
<td>kW</td>
</tr>
<tr>
<td>Cross-over energy requirement</td>
<td>Energy balance over the cross-over section. This value is the sum of the enthalpies of the cross-over output and the recycled blow-over, minus the chlorinator output enthalpy and the TiCl(_4) cooling enthalpy</td>
<td>kW</td>
</tr>
<tr>
<td>Actual off-gas CO/CO(_2) ratio</td>
<td>Molar ratio of CO to CO(_2) in the chlorinator output stream</td>
<td></td>
</tr>
</tbody>
</table>

### Table VIII

**Compounds used to describe the materials in the model, obtained from the FactSage 5.5 FACT pure substance database (Bale et al., 2009)**

<table>
<thead>
<tr>
<th>Gas</th>
<th>Liquid</th>
<th>Solid</th>
</tr>
</thead>
<tbody>
<tr>
<td>(FeCl(_2))(_2)</td>
<td>FeCl(_3)</td>
<td>Al(_2)O(_3). corundum(alpha)(s4)</td>
</tr>
<tr>
<td>(FeCl(_3))(_2)</td>
<td>HCl</td>
<td>Al(_2)O(_3). delta(s2)</td>
</tr>
<tr>
<td>(MgCl(_2))(_2)</td>
<td>MgCl(_2)</td>
<td>Al(_2)O(_3). gamma(s)</td>
</tr>
<tr>
<td>Al(_2)Cl(_3)</td>
<td>Cl(_2)</td>
<td>Al(_2)O(_3). kappa(s3)</td>
</tr>
<tr>
<td>AlCl(_2)</td>
<td>Cl(_2)</td>
<td>AlCl(_3). solid(s)</td>
</tr>
<tr>
<td>AlCl(_3)</td>
<td>Cl(_2)</td>
<td>C(_3). graphite(s)</td>
</tr>
<tr>
<td>Al(_2)Cl(_3)</td>
<td>Cl(_2)</td>
<td>CaCl(_2). hydrophilite(s)</td>
</tr>
<tr>
<td>AlCl(_3)</td>
<td>Cl(_2)</td>
<td>CaCO(_3). aragonite(s)</td>
</tr>
<tr>
<td>C(_2)Cl(_4)</td>
<td>O(_2)</td>
<td>CaCO(_3). calcite(s2)</td>
</tr>
<tr>
<td>C(_2)Cl(_6)</td>
<td>O(_2)</td>
<td>Ca(_3)O(_2). line(s)</td>
</tr>
<tr>
<td>AlCl(_3)</td>
<td>PCl(_3)</td>
<td>CaO(_2). solid(s)</td>
</tr>
<tr>
<td>Al(_2)Cl(_6)</td>
<td>PCl(_3)</td>
<td>C(_6)O(_3). solid(s)</td>
</tr>
<tr>
<td>Al(_2)Cl(_7)</td>
<td>SiCl(_4)</td>
<td>C(_6)O(_3). solid(s)</td>
</tr>
<tr>
<td>Al(_2)Cl(_8)</td>
<td>SiCl(_4)</td>
<td>C(_6)O(_3). solid(s)</td>
</tr>
<tr>
<td>AlCl(_3)</td>
<td>SnCl(_2)</td>
<td>C(_6)O(_3). solid(s)</td>
</tr>
<tr>
<td>Al(_2)Cl(_9)</td>
<td>SnCl(_2)</td>
<td>C(_6)O(_3). solid(s)</td>
</tr>
<tr>
<td>AlCl(_3)</td>
<td>ZnCl(_2)</td>
<td>C(_6)O(_3). solid(s)</td>
</tr>
<tr>
<td>Al(_2)Cl(_10)</td>
<td>ZnCl(_2)</td>
<td>C(_6)O(_3). solid(s)</td>
</tr>
<tr>
<td>AlCl(_3)</td>
<td>ZnCl(_2)</td>
<td>C(_6)O(_3). solid(s)</td>
</tr>
<tr>
<td>Al(_2)Cl(_11)</td>
<td>ZnCl(_2)</td>
<td>C(_6)O(_3). solid(s)</td>
</tr>
<tr>
<td>AlCl(_3)</td>
<td>ZnCl(_2)</td>
<td>C(_6)O(_3). solid(s)</td>
</tr>
<tr>
<td>Al(_2)Cl(_12)</td>
<td>ZnCl(_2)</td>
<td>C(_6)O(_3). solid(s)</td>
</tr>
<tr>
<td>AlCl(_3)</td>
<td>ZnCl(_2)</td>
<td>C(_6)O(_3). solid(s)</td>
</tr>
<tr>
<td>Al(_2)Cl(_13)</td>
<td>ZnCl(_2)</td>
<td>C(_6)O(_3). solid(s)</td>
</tr>
<tr>
<td>AlCl(_3)</td>
<td>ZnCl(_2)</td>
<td>C(_6)O(_3). solid(s)</td>
</tr>
<tr>
<td>Al(_2)Cl(_14)</td>
<td>ZnCl(_2)</td>
<td>C(_6)O(_3). solid(s)</td>
</tr>
<tr>
<td>AlCl(_3)</td>
<td>ZnCl(_2)</td>
<td>C(_6)O(_3). solid(s)</td>
</tr>
<tr>
<td>Al(_2)Cl(_15)</td>
<td>ZnCl(_2)</td>
<td>C(_6)O(_3). solid(s)</td>
</tr>
<tr>
<td>AlCl(_3)</td>
<td>ZnCl(_2)</td>
<td>C(_6)O(_3). solid(s)</td>
</tr>
<tr>
<td>Al(_2)Cl(_16)</td>
<td>ZnCl(_2)</td>
<td>C(_6)O(_3). solid(s)</td>
</tr>
<tr>
<td>AlCl(_3)</td>
<td>ZnCl(_2)</td>
<td>C(_6)O(_3). solid(s)</td>
</tr>
</tbody>
</table>
The first term in Equation [6], which is the maximum possible blow-over rate according to the mass balance, is derived as follows:

\[ F_{i=1} = F_{\text{feed},i} + F_{\text{bar},i} \]

The rate at which particles enter size class \( i \) \((F_{\text{in},i})\) is calculated as follows:

\[ F_{\text{in},i} = F_{\text{feed},i} + K_i \cdot A \cdot X_{\text{cr},i} + F_{\text{ret},i+1} \cdot \frac{V_i}{V_{i+1}} \quad [7] \]

The rate at which particles leave the larger size class \( i+1 \) \((F_{\text{out},i+1})\) due to chemical reaction is calculated as follows:

\[ F_{\text{out},i+1} = F_{\text{in},i+1} - F_{\text{bo},i+1} \quad [8] \]

The total blow-over rate of a feedstock is calculated as the sum of blow-over for all the particle size classes.

\[ F_{\text{bo}} = \sum_i F_{\text{bo},i} \quad [9] \]

The composition of the blow-over is derived from the composition of the feed materials. The above methodology is based on the following assumptions and simplifications:

➤ The composition of particles is that of the specified feed material, and is constant throughout each particle
➤ Particles are spheres and are evenly distributed throughout each size class
➤ Particles do not break, and the only cause of particles becoming smaller is chemical reaction.

**Implementation**

The model was implemented mostly in the Microsoft .NET environment with the C# programming language. Microsoft Excel® was used as the front end because it is widely available and used in industry. All thermochemical calculations were done using the ChemApp thermochemical library (Petersen and Hack, 2007) and data exported from FactSage (Bale et al., 2009).

**Validation**

The model was validated qualitatively through interviews with persons that have first-hand knowledge and experience of the chlorination process. Quantitative validation was planned, but was ultimately cancelled for corporate reasons.

**Modelling Studies**

**Value-in-use concepts**

Value-in-use (VIU) models combine technical and financial information to provide a decision-making tool for product assessment and customer interaction. The concept aims to extract maximum sustainable value through knowledge and understanding of the value chain for the customer and producer. One of the main uses of VIU models is to evaluate product changes against a base case and determine the financial impact of the change. VIU models can also be used to compare and assess the value of different products in a customer’s process. Examples where these two concepts have been practically used are provided in the following sections.

**Example 1: production cost versus customer benefit**

The first example evaluated the cost of producing a higher TiO₂ grade slag versus the savings incurred by chloride producers.

Ilmenite (FeTiO₃) is the most abundant titanium-bearing mineral and contains between 45 and 60% TiO₂ (Moodley, 2011). Ilmenite cannot be used directly in most pigment production processes and has to be treated in order to
upgrade the TiO₂ content. In the smelting process, which can take place in either an AC or a DC furnace, ilmenite is reduced using anthracite to produce pig iron and titania-rich slag.

Titania slag competes with natural rutile (NR), synthetic rutile (SR), and upgraded slag (UGS) as feedstock to the chloride pigment process. NR, SR, and UGS contain more TiO₂ units than the titania slag, which has a typical titania content of 85-87% TiO₂. Production of a higher TiO₂ slag using a conventional smelting process, although beneficial to the chloride pigment producers, incurs increased reductant and energy requirements, increased refractory wear, possible tapping issues, and foaming in the smelting furnace. There is an increasing demand for slag producers to produce higher TiO₂ content slag, since waste generation and chlorine costs are reduced.

Burger et al. (2009) utilized the chlorinator model together with a smelter VIU model to evaluate the viability of producing a 90% TiO₂ slag instead of the more conventional 85-87% TiO₂ slag. The chlorinator model has been described in detail in this paper. The smelter VIU model was developed to model the production of TiO₂ slag in a DC arc furnace. It is an Excel-based model that combines thermodynamic data and plant data to calculate the energy requirements, reductant requirements, and slag and metal yield for the smelter. This is combined with financial information to quantify the costs that the slag producer will incur to produce different quality slags.

Utilizing a higher TiO₂ feedstock in the chlorinator results in less waste generation, lower treatment and disposal costs, and lower chlorine consumption, hence it results in a saving for chloride pigment producers. However, producing a higher TiO₂ slag results in increased reductant and energy requirements, higher metal yield, and a lower slag yield. The chlorinator VIU model and a smelter VIU model were used to quantify the savings realized by the chloride producers and the extra costs incurred by the slag producer.

**Smelter model assumptions**

The following assumptions were made in the smelter model (Burger et al., 2009):

- All feed materials enter the reactor at 25°C
- Blow-over is determined by the elutriation constant, which was determined experimentally for different size fractions and different feedstocks
- Waste treatment includes neutralization of the waste with lime
- Chlorinator operating temperature is 1000°C
- The exit gas stream from the chlorinator is cooled to 200°C by liquid TiCl₄ sprays (below the sublimation point of ferric chloride)
- The molar ratio of CO/CO₂ in the gas product from the chlorination reactor is 1
- Price assumptions for the model are based on figures obtained from a TZMI (2007).

**Chlorinator model results**

In the base case, only an 85% TiO₂ slag is fed to the chlorinator. The percentage change in reagent consumption and waste generation is reported in Table XIV for the alternative case, *i.e.* when only a 90% TiO₂ slag is used in the process.
chlorinator. A negative value indicates that consumption is lower with the 90% TiO2 feedstock.

Figure 5 is a waterfall graph that shows the monetary contributions of coke, chlorine, logistics, and waste cost to the increase/decrease in value of the 90% TiO2 feedstock. The contribution is expressed as a percentage of the 85% TiO2 slag price (i.e. the base case). Chloride producers will utilize more coke to chlorinate a higher TiO2 feedstock, therefore petroleum coke will have the opposite effect of the chlorine and waste costs and reduce the value of the higher TiO2 feedstock as indicated in Figure 5. The impact of increased petroleum coke consumption is, however, low compared to the waste and chlorine savings. The overall VIU calculations indicate that the pigment producer’s costs will be 9.2% lower if a 90% TiO2 slag is utilized instead of an 85% TiO2 slag.

The study indicates that the cost of producing a high-grade slag outweighs the savings realized at the pigment plant. However, although production of a higher TiO2 slag is not viable based on the assumptions and prices used in the model, this could alter as prices change, and the use of VIU models will enable the changes to be quickly assessed.

Example 2: relative feedstock values

In the second example, the relative value of an 86% TiO2 feedstock is compared with a 95% TiO2 feedstock. Utilizing a higher TiO2 feedstock in the chlorinator results in less waste generation, lower treatment costs, lower disposal costs, and lower chlorine consumption, and hence results in a saving for chloride producers. The value of TiO2 feedstock containing more TiO2 units should therefore be higher. The chlorinator model was used to determine the relative value of using a titania slag (86% TiO2) compared to a natural rutile product containing 95% TiO2 in the chlorination process, considering the major cost elements (i.e. the costs of petroleum coke, chlorine, waste disposal and waste treatment).

Model assumptions

➤ Same as in Example 1
➤ Price assumptions are based on figures obtained from a TZMI (2012) and escalated to present-day prices.

Model results

The major results from the chlorinator VIU model are provided in Table XV. In the base case, only an 86% TiO2 slag is fed to the chlorinator. The percentage change in reagent consumption and waste generation is reported in Table XV for the alternative case, i.e. when only natural rutile is used.

With natural rutile, less waste is generated, and less lime and make-up chlorine is required, but coke consumption increases.

The waterfall graph (Figure 6) shows the monetary contribution of coke, chlorine, and waste cost to the increase/decrease in value of the natural rutile. The contri-

Table XIII
Summary of smelter VIU results (Burger et al., 2009)

<table>
<thead>
<tr>
<th>Parameter (per ton ilmenite)</th>
<th>Change from 85% to 90% TiO2 slag</th>
</tr>
</thead>
<tbody>
<tr>
<td>Slag yield</td>
<td>-5.5%</td>
</tr>
<tr>
<td>Metal yield</td>
<td>+7.2%</td>
</tr>
<tr>
<td>Electrode consumption</td>
<td>+3.1%</td>
</tr>
<tr>
<td>Energy consumption</td>
<td>+3.9%</td>
</tr>
<tr>
<td>Reductant consumption</td>
<td>+7.1%</td>
</tr>
</tbody>
</table>

Table XIV
Summary of chlorinator VIU results

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Change from 85% to 90% TiO2 slag</th>
</tr>
</thead>
<tbody>
<tr>
<td>Petroleum coke consumption</td>
<td>+3%</td>
</tr>
<tr>
<td>Chlorine gas consumption</td>
<td>-7%</td>
</tr>
<tr>
<td>Lime consumption for neutralization</td>
<td>-24%</td>
</tr>
<tr>
<td>Waste generated</td>
<td>-24%</td>
</tr>
</tbody>
</table>
bution is expressed as a percentage of the 86% TiO₂ slag price (i.e. the base case).

VIU calculations show that for the given set of assumptions and prices, the value of natural rutile in the chlorinator is 6.7% higher than that of the slag. This is largely due to the chlorine costs, which account for 4.80% of the 6.7% change. In the Burger et al. (2009) study, the contribution from waste treatment costs (Figure 5) was the highest, but due to the decrease in waste treatment costs (TZMI, 2012), the chlorine costs are now the major cost driver.

Knowledge of the relative value of the feedstocks is important for suppliers to position themselves in the market and understand the value of their feedstock.

Conclusions

Modelling of the chlorination process facilitates the quick assessment of different feedstocks and provides valuable insight into a process that feedstock producers normally do not have access to.

Although VIU models are a powerful decision making tool, care must be taken to ensure that the assumptions are valid and are regularly updated.

References


Interaction of dust with the DC plasma arc – a computational modelling investigation

by Q.G. Reynolds*

Synopsis
The presence of dust and fume suspended in the freeboard region is a common feature of the operation of direct current (DC) plasma smelting furnaces. This occurs primarily as a result of the use of fine feed materials together with the open-arc, open-bath operation of such smelters, and is exacerbated by the high velocities and turbulent mixing of the gas in the vicinity of the arc jet. Dust and fume losses into the furnace off-gas system can be significant in some cases and may have economic, operational, and environmental impacts on the process. A computational modelling study is presented in which the concentration of dust material was considered as a continuous field subject to a governing partial differential equation. Settling behaviour was calculated as a function of particle size, local gas/plasma temperature, and other physical properties. Development of the coupling between the concentration field and a magnetohydrodynamic description of the arc is shown, and the resulting models were used to compute various aspects of the behaviour of the concentration field in the arc region for a variety of furnace conditions. Time-averaged as well as transient models of the arc were used to generate the results presented. Qualitative case studies produced several practical suggestions for furnace operation, including increased dust capture by the bath when feed ports are located closer to the electrode, and the possible effects of feed segregation in the furnace freeboard based on dust particle size and density.

Keywords
DC furnace, arc plasma, dust entrainment, continuum computational model, freeboard flow, arc flow.

Introduction
The direct current (DC) arc furnace is employed as a metallurgical unit operation in a significant portion of the pyrometallurgy industry worldwide. While DC furnaces are traditionally used in the re-melting of steel scrap, they are becoming increasingly attractive for the smelting of raw materials to produce commodities such as ferrochromium, ilmenite, ferronickel, platinum group metals, magnesium, and others (Jones and Curr, 2006).

The layout of a typical DC furnace is shown in Figure 1. A cylindrical shell topped with a conical roof and lined with refractory materials forms the furnace vessel, and contains the molten process material. This molten bath typically consists of multiple liquid phases, with oxide (slag), alloy, and/or sulphide (matte) phases possible. Raw materials consisting of ores, reductants, and chemical modifiers are continuously fed into the vessel via feed ports at various locations in the roof. Single or multiple pre-baked graphite electrodes enter through the top of the roof. A power supply consisting of a transformer connected to a DC rectifier feeds electrical power to the furnace via the graphite electrode and an anode connection in the hearth.

The electrical energy is converted into thermal energy in the plasma arc, which is the primary heating and stirring element inside the DC furnace. The arc consists of ionized freeboard gas containing a mixture of ions and free electrons, and is able to conduct electricity well. The electromagnetic forces interact with the plasma gas to accelerate and heat it, resulting in the formation of the arc – a high-temperature, high-velocity jet directed at the surface of the molten bath (Bowman, 1994). The arc may be thought of as the ‘engine room’ of the furnace, and improving the understanding of the physical behaviour of this region is invaluable for the improvement of current and future furnace designs.

One of the cited advantages of using DC furnaces for a particular process is that it is able to treat very fine materials directly, without the need for an agglomeration or briquetting stage prior to their introduction into the furnace (Jones and Curr, 2006). While it simplifies the furnace plant and operation considerably, this practice often raises the issue of dust carry-over – that is, how much of the dust from the feed material bypasses treatment in the furnace and is carried out of the off-gas ducts by entrainment in the gas flow. This is exacerbated in DC furnaces by the open-bath, open-arc nature of the operation, which provides no physical obstruction to the flow and circulation of gas in the freeboard.

Computational study of the dust behaviour in DC furnaces may be broken down into two...
Interaction of dust with the DC plasma arc – a computational modelling investigation

broad areas – the freeboard flow problem and the arc flow problem. In the freeboard flow problem, one models the large-scale flow structures inside the entire furnace freeboard space and uses these models to predict dust bypassing from the feed port inlets to the off-gas outlets. In order to maintain computational economy, these models generally either ignore the presence of the arc or treat it as a simple jet, and use simplified fluid descriptions for the gas. A number of researchers have done valuable work in this area, predominantly focusing on engineering applications inside and around furnaces (de Jong and Mitchell, 2010; Ravary and Gradahl, 2010). In the arc flow problem, the influence of the plasma arc on the entrained dust in its immediate vicinity is modelled in detail. This generally requires a more sophisticated mathematical description of the arc in terms of magnetohydrodynamics (e.g. Szekely et al., 1983). The coupling between the entrained dust and the plasma gas must also be accounted for, and may be added to such arc models by modelling the dust particles’ presence in several different ways, including continuum methods (Ranz et al., 1960) and particle methods such as discrete element modelling (Hager et al., 2013). Owing to the large driving forces and highly dynamic nature of the plasma arc, which can evolve on time scales of the order of milliseconds or less (Reynolds et al., 2010), study of the arc flow problem generally requires transient solution methods on high-resolution numerical meshes, and is considerably more computationally demanding even when considering only a small region of the freeboard space around the arc. As a result, it appears that little work has been done in the area to date.

In the present study a continuum computational model of the arc and dust concentration field is proposed, together with a discussion of various levels of coupling between the dust field and the arc plasma gas. The model is then used to examine the effect of various parameters on the dust distribution in and around the arc on a simplified, approximate two-dimensional geometry.

Model development

Equations describing the coupled momentum, energy, and electromagnetic fields are required in order to produce mathematical and computational models of plasma arcs. These have been described in some detail elsewhere (Reynolds et al., 2010), and are reproduced below.

\[
\frac{\partial (\rho U)}{\partial t} + \nabla \cdot (\rho U U) + \nabla P = \nabla \cdot \tau_{ij} + j \times B
\]

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho U) = 0
\]  

\[
\frac{\partial (\rho h)}{\partial t} + \nabla \cdot (\rho U h) = \nabla \cdot \kappa \nabla h + \frac{j \cdot j}{\sigma} + \nabla \left( \frac{5k_b}{2eC_p} \right) h - Q_R
\]

\[
j = \sigma (-\nabla \phi + U \times B)
\]

\[
\nabla \cdot j = 0
\]

\[
\nabla \times B = \mu_0 j
\]

The Navier-Stokes and continuity equations [1] represent the conservation of momentum and mass respectively. In Equation [1], \( \rho \) is the plasma density, \( U \) is the velocity vector, \( P \) is the pressure field, \( \tau_{ij} \) is the viscous stress tensor (Newtonian fluids with viscosity \( \mu \) are used in the present work), \( j \) is the electric current density vector, and \( B \) is the magnetic field vector.

The conservation of energy is governed by Equation [2]. In this relationship, \( h \) is the enthalpy of the plasma, \( \kappa \) is the thermal conductivity, \( C_p \) is the heat capacity, \( \sigma \) is the electrical conductivity, \( k_b \) is the Boltzmann constant, \( e \) is the electron charge, and \( Q_R \) is the radiation emission coefficient. The last three terms on the right-hand side of Equation [2] represent energy generation by ohmic heating, electron enthalpy transport, and energy loss from the plasma by radiation.

Maxwell’s equations for electrostatics and magnetostatics (Equation [3]) govern the electromagnetic fields in the plasma. Here, \( \phi \) is the scalar electric potential field, and \( \mu_0 \) is the magnetic permeability of free space.

Under the assumptions of local thermodynamic equilibrium (Boulos et al., 1994), it is possible to describe the plasma fluid using a single temperature \( T \). Enthalpy and all physical properties of the plasma are strongly temperature-
interaction of dust with the DC plasma arc – a computational modelling investigation

dependent, and are therefore treated as variables in Equations [1]–[3]. This temperature dependence, together with the additional coupling via convection and source terms, results in a fully-coupled system in which all field variables depend to some degree on the others.

Modelling the dust field

In order to evaluate the distribution of dust in the arc region, a continuum approach is taken. If the local mass concentration of dust, \( c \) (mass of dust per unit mass of plasma gas), is taken as a field variable, then an additional transport equation for the mass conservation of dust may be written as shown in Equation [4].

\[
\frac{\partial (\rho c)}{\partial t} + \nabla \cdot (\rho (U + U_S)c) = \nabla \cdot D_D \nabla (\rho c) \tag{4}
\]

Here, \( U_S \) is the terminal settling velocity of the dust particles in stagnant plasma gas, and \( D_D \) is a diffusion coefficient for the dust field. An assumption has been made in order to derive Equation [4], namely that the dust particles are fully entrained at the same velocity as the plasma gas at all times apart from the additional settling velocity. This implies that the dust particles are accelerated or decelerated to the local plasma gas velocity instantly, without any time lag due to the action of drag forces.

\( U_S \) may be calculated from the Stokes settling law (Lamb, 1932) as shown in Equation [5], assuming that the dust particles are sufficiently small that the Reynolds number remains below 1; this is generally the case for particles less than 1 mm in size falling through plasma gases.

\[
U_S = \frac{(\rho_D - \rho)gd_D^2}{18\mu} \tag{5}
\]

Here, \( \rho_D \) and \( d_D \) are the dust particle density and average diameter respectively, and \( g \) is the vector of acceleration due to gravity.

\( D_D \) is somewhat harder to calculate accurately as it is generally a function of both molecular diffusion due to Brownian motion and collisions with particles in the plasma gas, and turbulent diffusion due to the eddy viscosity of the surrounding fluid. The molecular component may be estimated using the Stokes-Einstein relationship (Einstein 1905), shown in Equation [6].

\[
D_{D,M} = \frac{k_B T}{3\pi \mu d_D} \tag{6}
\]

Evaluation of this equation for a range of typical plasma gas conditions gives values for \( D_{D,M} \) of between \( 10^{-10} \) and \( 10^{-12} \) m\(^2\)/s. These are so low as to be negligible, and the molecular diffusivity may be safely ignored.

In the case of the fully-transient and coupled dust models, in which Equation [4] is solved in lock-step with Equations [1]–[3], no turbulence closure model is used, and the solution is obtained on high-resolution meshes which attempt to resolve the majority of the turbulent flow scales directly. For these cases, the eddy diffusion component is calculated explicitly as part of the flow field and \( D_D \) may be taken as equal to \( D_{D,M} \). However, in the case of time-averaged models with decoupled solution of the dust field (as are used for many of the results presented later), the turbulent eddy viscosity is not calculated directly and must be estimated from the time-averaged velocity field. For this purpose, the strain rate relationship familiar from large eddy simulation methods (Smagorinsky, 1963) is used, as shown in Equation [7].

\[
D_{D,T} = \nu_T = (C_S \delta)^2 |\mathbf{S}| \tag{7}
\]

Here, \( \mathbf{S} \) is the strain rate tensor, which may be determined from the velocity field. \( \delta \) is a length parameter representing the size of the numerical mesh elements at any given location, and \( C_S \) is a dimensionless empirical constant with value 0.16 – 0.2. Evaluation of Equation [7] gives a turbulent diffusivity field, and the total diffusivity to be used in Equation [4] may be calculated from \( D_D = D_{D,M} + D_{D,T} \).

Coupling between dust, energy, and momentum fields

It is important to note that Equations [1]–[4] represent a system with only one-way coupling between the dust concentration field and the remaining variables. The arc affects the dust concentration distribution, but not vice versa. Such decoupling is valid for low dust concentrations, and has certain advantages; for example, in cases in which the settling velocity of the dust is very low, the time scales of the motion and evolution of the dust field may differ from those of the arc by an order of magnitude or more. In such cases, it is convenient to calculate time-averaged representative flow and temperature fields from Equations [1]–[3], and then solve Equation [4] separately using the time-averaged fields to study the evolution of \( \rho c \).

In general, however, the presence of a dust concentration field distributed through the plasma gas will affect both the momentum and heat transfer behaviour via two-way coupling. In order to study this effect, a simplified method of coupling is adopted based on the assumption of thermal and momentum equilibrium – that is, that the local temperature and velocity (apart from settling) of the dust particles are identical to those of the plasma gas. In reality, the dust particles have their own velocity and temperature distributions, with momentum and energy exchanged between them and the plasma gas resulting in acceleration and heating of the dust. However, this would not only introduce two additional fields requiring numerical solution (dust velocity and temperature) but also raise additional questions of how the transport between dust and plasma gas is to be modelled. As the purpose of the present study is to examine the gross qualitative effects of coupling between dust and arc, the simpler equilibrium approach was deemed justified, but this remains an open area for future work.

Under the equilibrium assumption for momentum, neglecting any additional momentum transfer to the plasma due to settling of the dust, and using the approximation that \( D_D = D_{D,M} = 0 \) in the fully-coupled model, additional source terms representing the momentum of acceleration and deceleration of the dust field are included in the Navier-Stokes Equation [1] to give:

\[
\frac{\partial (\rho U)}{\partial t} + \nabla \cdot (\rho(UU)) + \left[ \frac{\partial (\rho c U)}{\partial t} + \nabla \cdot (\rho c U U) \right] \tag{8}
\]

\[
+ \nabla P = \nabla \cdot \mathbf{S}_f + \mathbf{j} \times \mathbf{B}
\]
Interaction of dust with the DC plasma arc – a computational modelling investigation

Similarly, under the equilibrium assumption for energy, source terms are added to Equation [2] to account for the transport of thermal energy contained in the dust field. Some re-arrangement and simplification using Equation [4] then leads to:

\[
\frac{\partial (\rho h)}{\partial t} + \nabla \cdot (\rho \mathbf{U} h) + P_c \frac{\partial h}{\partial t} + (\mathbf{U} + \mathbf{U}_s) \cdot \nabla h = \frac{\kappa}{\sigma} \nabla h + \frac{j \cdot j}{\sigma} + \nabla \left( \frac{5 k B h}{2 e C_p} h \right) - Q_k \quad \text{[9]}
\]

Here, \(C_p\) is the heat capacity of the dust particles, assumed to be constant.

Two-way coupling between the dust concentration field and the arc’s momentum and enthalpy fields may then be realized by solving Equation [8] in place of Equation [1], Equation [9] in place of Equation [2], or both.

Model geometry and boundary conditions

While the model as developed extends naturally to both two- and three-dimensional cases, only 2D cases were considered in the present study. Time and resource limitations were the main reason for this, as the solution of high-resolution transient models of the plasma arc in three dimensions is extremely computationally intensive and time-consuming.

In order to study representative behaviour of the arc and associated dust fields, a 2D planar model region is generated by taking a slice through the centre line of the arc. Axisymmetry is not enforced in the model, and while this allows asymmetric structures and phenomena to evolve naturally, it is important to note that the planar nature of the model may be expected to result in some discrepancies between real three-dimensional furnaces and the model results. Such models should therefore best be viewed as ‘arc-like systems’ which are capable of generating physically realistic and qualitatively similar behaviour, rather than quantitatively accurate engineering tools (Reynolds et al., 2010). The purpose of the present study is primarily qualitative, and the 2D approach was deemed to be an acceptable approximation.

The geometry used for the arc flow models is shown in Figure 2.

ABCD describes the surface of the molten bath, which acts as the anode in the system. In general, the thrust force of the arc deforms the bath surface, creating a cavity BC below the electrode tip. The graphite electrode surface is described by FGHJKLM, with the cathode attachment spot J acting as the cathode and the root of the plasma arc jet. All other boundaries are open to the freeboard atmosphere, permitting inflow and outflow of plasma gases and dust. NO is the dust inlet, through which a fixed concentration of dust is introduced into the arc region.

Boundary conditions for the various fields in the model are required in order to complete the solution. These are shown in Table I.

Here, \(P_0\) is the gas pressure in the furnace freeboard, typically atmospheric. \(h_A\), \(h_O\), and \(h_E\) are the plasma gas enthalpies at the anode surface temperature (taken as 5000K), inlet freeboard gas temperature (taken as 5000K), and electrode surface temperature (taken as the sublimation temperature of graphite, 4100K) respectively. \(c_0\) is the inlet dust concentration, fixed for each simulation. \(j_0\) is the current density at the cathode spot, for which a value of \(3.5 \times 10^7\) A/m\(^2\) was used (Bowman, 1994).

Specifying the total current carried by the arc permits the calculation of the diameter of the cathode spot \(x_p\), using the given value of \(j_0\). Knowing the current and the distance from the cathode tip to the surface of the anode also permits the calculation of the thrust force generated by the arc (Bowman, 1994) and by analogy with turbulent gas jets, the shape and dimensions of the cavity surface BC (Cheslak et al., 1969). BC is treated as static in the present model. However, in general this zone will be characterized by a large amount of turbulent splashing and mixing. This would be expected to significantly enhance dust capture by the bath in this area, but a detailed examination of this phenomenon is left for future studies.

Numerical and computational implementation

In order to obtain numerical solutions of Equations [1]–[3] as well as the fully-coupled systems using Equations [8] and [9], a custom solver application was written in C++ code using the open source OpenFOAM v2.3.0 framework for field solutions of differential equations (OpenFOAM, 2014). OpenFOAM implements a generalized unstructured-mesh finite-volume method for defining conservation equations, and provides a number of accelerated and parallelized matrix solution techniques suitable for such problems.

Following the general approach of Sass-Tisovskaya (2009), an existing OpenFOAM CFD solver for incompressible flow using the Pressure Implicit with Splitting of Operators (PISO) predictor-corrector algorithm was heavily extended and modified to allow for general temperature-dependent plasma physical properties specified via lookup tables. Additional solvers for enthalpy and the electromagnetic fields were then constructed from scratch and incorporated into the standard PISO algorithm used for the velocity and pressure field solutions. Finally, a solver for the dust equation [4] was constructed and added to the algorithm, together with runtime switches to enable user activation or deactivation of the coupling behaviour.

Computational meshes for the problems were constructed and parsed into OpenFOAM format via Perl scripts using Gmsh v2.5.1 (Gmsh 2014), an open source geometry and mesh generation application. The solver code was compiled and executed on a small computational cluster running Ubuntu Linux 12.04 LTS. GCC 4.6.3 (GCC, 2014) was used as the compiler, along with standard OpenFOAM wmake scripts. OpenMPI was used as...
Interaction of dust with the DC plasma arc – a computational modelling investigation

Results

Effect of the arc on the dust – one-way coupling

In order to study the effect that the flow field of the plasma arc has on the dust concentration field in the model region, a decoupled approach using time-averaged fields was taken. The procedure was as follows:

- Set up the model geometry and parameters
- Run the plasma arc model (Equations [1]–[3]) with no dust present for a short time period, until the initial conditions have decayed
- Generate time-averaged velocity and temperature fields using the results of the initial run
- Run the dust transport model (Equation [4]) for an appropriate length of time to study the evolution and development of the dust concentration field to steady state.

Base case model

As a starting point for the one-way coupling study, a base case was defined. From this initial starting point, the sensitivity of the model to various design and material parameters could be studied. The parameters used for the base case model are shown in Table II. Dimension subscripts refer to Figure 2.

The dimensions of the region were chosen to match a typical small-scale pilot plant DC arc furnace facility. For the base case model, the dust inlet was located equidistant between the electrode and the edge of the model region. Dust concentrations in smelting furnace freeboards typically range between 0.1 and 1 kg/kg (Geldenhuys and Jones, 2009), and the diameter of suspended and bypassed dusts has been measured between 20 and 1000 µm (Guezennec et al., 2005; Rughubir and Bessinger, 2007). Tabulated physical properties as functions of temperature for air thermal
Interaction of dust with the DC plasma arc – a computational modelling investigation

plasmas were used (Boulos et al., 1994). The plasma arc model with no dust present was used to compute the first 100 ms of arc motion, with the final 25 ms being used for time averaging. The time-averaged fields were then used as input for the dust model, which was run for an additional 100 ms. An unstructured mesh of approximately 20 000 quadrangular elements was used for the simulations, in which high resolution was applied in regions of high shear and energy flux.

Time-averaged velocity and temperature fields of the arc are shown in Figure 3. It can be seen that time averaging of the rapid turbulent and chaotic dynamics of the arc column acts to produce a wide, conical temperature and jet velocity field which spreads out from the electrode tip into the space below. Figure 3b also shows the path of streamlines (in brown, including the settling velocity $U_s$) from the dust inlet at top left through the region and eventually out at the left boundary. It can be seen that the recirculation vortices generated around the arc result in substantial deformation of the streamlines, and much of the dust introduced at the inlet boundary is therefore likely to be entrained into the body of the arc jet.

Development of the dust concentration field $c$ for the base case model is shown in Figure 4. It can be seen that the dust is very rapidly drawn into the high-velocity arc jet within 10 ms of entering the region. The fully developed steady-state dust concentration profile is shown in Figure 4d, with the majority of the dust passing through the arc jet before being carried out of the region by the strong flow adjacent to the bath surface. A smaller portion of the dust is captured by the bath surface.

The rate of dust convection or settling through the various boundaries can be studied by calculating the dust mass flux at the boundary surface (per linear metre in the y-direction, since the model domain is planar). Figure 5 shows the evolution of the rate of dust ingress or removal through the inlet (surface NO in Figure 2), bath (surface ABCD in Figure 2), sides (surfaces DE and AP in Figure 2), and top (surfaces EF, MN, and OP in Figure 2). The inlet flux is seen to be constant, as expected, while the dust fluxes through the various boundaries rise from zero to their steady-state values between 8 and 20 ms.

Once steady state is reached in the base case model, approximately 17% of the dust entering the region through the inlet is captured by the bath in the vicinity of the arc, 77.4% is bypassed out the sides of the region (mostly very close to the bath surface), and 5.6% recirculates back into the freeboard space above the arc region.

Figure 3 – Plot of time-averaged (a) temperature and (b) velocity unit vector fields, base case parameters

Figure 4 – Dust concentration field at various times, base case model. Scale 0 (grey) to 0.5 (black) kg/kg
Effect of arc length

In order to study the effect of arc length (distance from tip of electrode to bath surface) on the dust transport model, several cases were set up and run keeping all parameters in Table II constant, with the exception of $z_H$ which was varied between 0.025 m and 0.2 m. Arc models were run for 100 ms (with 25 ms time-averaging) in order to generate averaged temperature and velocity fields. The dust transport model was then run for 100 ms for each case.

The resulting steady-state dust concentration fields for the two extreme cases are shown in Figure 6. It is immediately obvious that running at shorter arc lengths results in far less entrainment of dust. This is primarily due to the reduction in size of the high-velocity recirculation zones around the arc – these zones scale in proportion to the length of the arc jet, and shorter arcs produce more compact velocity fields. Short arcs also produce a narrower, deeper cavity in the bath surface, which redirects much of the impinging gas flow back into the arc jet. As a result, dust is able to settle most of the way to the bath surface before interacting with the velocity field to any noticeable degree. The opposite is true for long arcs – these create very large vortex cells on either side of the arc jet, and the dust is almost immediately drawn into the body of the arc as it enters the region.

The dispersion of dust from the inlet to the boundary surfaces at steady state for the various arc length cases is shown in Figure 7. Increasing the arc length shows a general trend of increasing the dust bypassed out of the arc region, either via the side or top boundaries. Shorter arc lengths produce less bypassing and permit more capture of the dust by the bath, assuming all other geometry and material parameters remain constant.

Effect of arc current

The electric current carried by the arc is a key design and operation variable for DC furnaces. The effect of current on the dust behaviour was examined by varying the specified DC current while keeping all other parameters of the model as listed in Table II constant. Currents from 250 to 2000 A were used. Run-times for the arc model and time-averaging step varied from 400 ms (100 ms averaging) in the 250 A case to 50 ms (12.5 ms averaging) in the 2000 A case. The dust transport models were run for an additional 100 ms, sufficient for the fields to evolve to steady state in all cases.

Steady-state dust concentration fields for the 250 A and 2000 A cases are shown in Figure 8. While both high and low currents show some degree of entrainment of dust into the arc jet and significant bypassing of dust material out of the region boundary at left, it can be seen that the lower velocities resulting from lower currents result in more pronounced settling of the dust cloud as it is convected. The higher currents, while entraining more of the dust and carrying it closer to the bath surface, result in such high velocities that the dust is rapidly carried out of the side of the model region before it gets a chance to settle onto the bath surface.

The steady-state dispersion of the inlet dust to various boundaries for the different arc current cases is shown in Figure 7.
Interaction of dust with the DC plasma arc – a computational modelling investigation

Figure 8 – Steady-state dust concentration fields at various currents. Scale 0 (grey) to 0.5 (black) kg/kg

Figure 9 – Distribution of dust flux as a function of current

Figure 9. These results are somewhat noisy and it is difficult to discern an overall trend in the deportment of the dust flux, although comparing the result at 500 A to that at 1000 A suggests the possibility that higher currents may cause more dust to be bypassed out of the arc region. This may be expected given the fact that increasing current typically increases the velocities of the plasma in the arc (Reynolds et al., 2010), significantly reducing the residence time of the dust in the arc region and therefore reducing the time available for it to settle as it passes through.

Effect of dust inlet location

The location of the dust inlet, although a somewhat artificial concept in the present model, may be related back to the design of feed systems for DC furnaces and in particular the location of the feed ports in the furnace roof. With this in mind, the location of the inlet was varied while keeping all other parameters constant. Cases with the dust inlet adjacent to the electrode, and at the edge of the region, were examined. As before, arc models with no dust present were run for 100 ms, with the last 25 ms being used to generate time-averaged fields for input into the dust transport model, which was then run for an additional 100 ms.

Steady-state dust concentration fields resulting from changing the location of the dust inlet are shown in Figure 10. It is interesting to note that moving the dust inlet does not affect the gross dust entrainment behaviour, namely that the falling dust column is drawn into the arc jet along the electrode surface at the centre of the furnace, accelerated toward the bath surface, and then convected outward. However, it can be seen that in the case of the adjacent inlet considerably more of the dust is captured by the bath surface before it leaves the model region.

This effect is quantified in Figure 11, showing dispersion of the dust to various boundaries in the model at steady state. Location of the dust inlet close to the electrode results in far more efficient dust capture by the bath in the vicinity of the arc, with more than 95% settling to the bath surface in this case. As the inlet is moved further away, the dust has greater opportunity for interaction with recirculation structures in the plasma gas around the arc column, and as a result a much larger fraction of the incoming dust is captured into these recirculation structures and convected out of the side and top boundaries.

Effect of dust density

In general a dust stream entering a DC furnace as part of the raw material feed will be polydisperse, that is, it will consist of a distribution of particle types and sizes. It is therefore of some value to examine the effect of changing the dust properties, which affect the settling velocity $U_s$, on the dust behaviour in the model. Dust density may be taken as a crude proxy for the composition of the particles – low densities of the order of 1500 kg/m$^3$ are typical for carbonaceous reductants, while higher densities of 7000 kg/m$^3$ or more are common for metallic components in the furnace feed. Different densities were tested in the model while keeping all other parameters constant as per the base case. The standard 100 ms arc time-averaging calculation with 25 ms of averaging was used, together with an additional 100 ms run time for the dust transport model.

Figure 12 shows the steady-state dust concentration profiles in the arc region for a low-density and a high-density dust.

It can be seen that the low-density dust with its lower settling velocity remains largely contained in the recirculation cell near to the electrode surface – very little dust actually enters the arc column. In contrast, the high-density dust settles through the recirculation layer but is then strongly convected toward the side of the model region.

Distribution of the dust flux over the various boundary surfaces in the models at steady state is shown in Figure 13. Lower density components in the dust stream were seen to remain entrained in the velocity field of the arc as they pass through the model region. In extreme cases, the low-density material may be circulated out of the top of the region and back into the freeboard space above. Generally, higher density components will still experience significant entrainment and bypassing, but they will tend to be carried out of the sides of the arc region close to the bath surface and
are likely to settle out rapidly as the arc's velocity field decays away from the electrode.

Effect of dust particle diameter

The polydisperse nature of the dust stream entering the arc region extends to particles of different diameter. This can drastically affect the dust behaviour in the region, as settling velocities scale with the square of the diameter as per Equation [5]. The dust transport model was used to examine the behaviour of a variety of dust particles with diameters ranging from 50 $\mu$m up to 1250 $\mu$m. As before, all other parameters as per Table II were held constant, with only the dust diameter $d_D$ varying. 100 ms time-averaging runs to calculate the arc flow and temperature fields were used as before, together with additional 100 ms runs for each diameter model case.

Figure 14 shows the dust concentration fields at steady state for particles at the two extremes of size. Substantial differences are obvious; the smaller particles, unable to settle fast enough to overcome the recirculation flow that the arc creates in the surrounding plasma gas, are immediately entrained and convected out of the arc region by the medium-velocity gas flow near to the electrode. The larger particles, with much higher settling velocities, pass easily through the recirculation regions before being drawn toward the arc by the high-velocity flow in the vicinity of the main arc jet.

The distribution of the dust fluxes on the model boundary surfaces at steady state are shown as a function of the dust particle diameter in Figure 15.

A distinct trend may be observed in the data, with smaller particles being so easily entrained by the flow patterns in and around the arc that they are completely bypassed out of the upper boundary of the region by convection. As the particle size increases past 500 $\mu$m, an increasing amount of dust is able to reach and settle on the bath surface, and the quantity convected through the top boundary drops away rapidly.

For a furnace feed stream containing dust across a wide range of size fractions, these differences in behaviour may result in substantially different fates for the different sizes.

![Figure 10 – Steady-state dust concentration fields for various inlet locations](image)

![Figure 11 – Distribution of dust flux as a function of inlet location](image)

![Figure 12 – Steady-state dust concentration fields for various dust densities](image)

![Figure 13 – Distribution of dust flux as a function of dust density](image)
Interaction of dust with the DC plasma arc – a computational modelling investigation

Smaller particles will tend to become suspended in the freeboard gas and lost via the furnace off-gas system, while larger particles may be entrained into the arc region temporarily but will ultimately be captured by the bath surface or furnace sidewalls, possibly some distance from the arc itself.

Effect of the dust on the arc – two-way coupling

In order to study the feedback effects of the dust interacting with the plasma arc, the fully-coupled dust-arc model is used. Since for these cases the dust transport equation [4] cannot be decoupled from the plasma arc equations [3], [8], and [9], a single unified model algorithm is used to solve the momentum, energy, electromagnetic, and dust fields simultaneously. This improves the level of detail and temporal accuracy of the model results, but at the cost of significantly increased computational complexity and longer run-times.

Effect of coupling terms

For the initial study, base case parameters were kept identical to those used for the one-way coupling cases (Table II). The only additional parameter required for the two-way coupling case was an indicative heat capacity for the dust particles, which was taken as 1100 J/kgK for the typical oxide materials found in metallurgical ores. This value is approximated as constant across the range of temperatures typically encountered in plasma arcs, although in reality the dust particles would be in a molten or gaseous state at the higher temperatures.

The effect of introducing different degrees of coupling was examined by starting with the model base case with no coupling, i.e. Equations [1]–[4], followed by cases with energy coupling only (Equations [1], [3], [4], and [9]), momentum coupling only (Equations [2], [3], [4], and [8]), and finally the fully coupled system. Each case was run for 100 ms of model time, using as initial conditions the established velocity, temperature, and electromagnetic fields from an earlier run of the arc model without any dust present.

Some example images showing the instantaneous temperature and dust concentration fields at the same time for each case are shown in Figure 16. It can be seen that although identical model parameters and initial conditions were used, activating various coupling terms results in the fields in the model producing very different patterns later in the simulation. Inspection of the general shape of the dust concentration field suggests that energy coupling has a relatively small effect, whereas momentum coupling changes the dust distribution patterns to a greater degree. Activating both coupling terms results in a visibly more turbulent and chaotically mixed dust concentration field, suggesting that there is increased transient behaviour of the flow and energy fields. This indicates that the presence of dust in the arc is able to affect its stability detrimentally in the model, by causing larger and more rapid fluctuations in the velocity and temperature fields.

This observation is borne out more quantitatively by examining the time dependence of the peak temperature, peak velocity, arc voltage, and dust flux at the bath surface for the various model cases. These results are shown in Figure 17. By comparing the solid grey line (one-way coupling only) on the graphs to the others, particularly the solid black line (full coupling), it can be seen that while the coupling terms are not large enough to appreciably change the average values of the fields over long time periods, they do significantly affect the variability of the fields over shorter periods. The arc model with full coupling is noticeably less stable than the model with one-way coupling only.

The entrainment of dust into a plasma arc may therefore be expected to produce an increase in high-frequency electrical noise in the furnace circuit, as well as an increased probability of arc extinction, due to the interaction between the dust and the arc.

Effect of dust inlet concentration in fully coupled model

In contrast to the one-way coupling case, the dust transport model in the fully coupled case is not linear due to the interaction terms in the momentum and energy equations. Therefore, the inlet dust concentration is able to affect the system behaviour in different ways – low concentrations would be expected to result in minimal effects, high concentrations in exaggerated effects. This was studied in the model with full coupling by varying the dust inlet concentration.

Figure 14 – Steady-state dust concentration fields for various dust particle diameters. Scale 0 (grey) to 0.5 (black) kg/kg

Figure 15 – Distribution of dust mass flux as a function of dust particle diameter

The Journal of The Southern African Institute of Mining and Metallurgy
while keeping all other parameters constant, and examining
the evolution of the various fields over time.

Visualizations of the dust concentration and temperature
fields at different times in the models are shown in Figure 18.

The visualizations demonstrate that while the various
fields in the fully coupled model start out with very similar
distributions in space, different behaviour evolves as soon as
the dust cloud begins to interact with the arc between 5 and
10 ms into the simulation.

There is considerable turbulent mixing by the high-
velocity flow in and around the arc jet in both cases, but it is
interesting to note that in the high-concentration case the arc
jet is occasionally deflected away from the dust inlet at an
angle of 45° or more (e.g. Figure 18d, c.f. Figure 18b). This
deflection is a transient phenomenon, but is observed to occur more frequently during the high-concentration case. A possible explanation for this behaviour is that as the dust concentration increases, it forms a physical and thermal barrier for the arc plasma due to the two-way coupling in the model. This results in the arc seeking the path of least resistance, deflecting away from the ‘cold wall’ that the falling column of dust represents.

The time dependence of the peak temperature, peak velocity, arc voltage, and dust flux at the bath surface for the different dust inlet concentration cases is shown in Figure 19.

It can be seen – especially in the arc voltage and dust flux graphs – that increasing the dust inlet concentration produces greater fluctuations relative to the mean value in the fully coupled model over the course of the 100 ms simulation period. This indicates that more extreme and violent changes
are occurring in the morphology of the fields that define the plasma arc. Together with the deflection behaviour observed, this would suggest that furnaces operating with high dust concentrations in the freeboard gas are likely to exhibit somewhat more instability and possibly even difficulties with arc extinction.

It is interesting to note that while both the average and peak arc voltages predicted by the high-concentration case are somewhat higher than those of the low-concentration case, it is a weakness of the present model that the effect is smaller than might be expected. From observations of real furnaces, the introduction of feed (together with dust) into the freeboard generally results in a significant increase in the resistance of the arc by both cooling of the plasma and increased turbulent flow.

Conclusions
Development of a continuum model for dust transport in the arc region of DC plasma arc furnaces was largely effective. The coupling between the governing equations of the plasma arc and the dust concentration field was developed in detail for cases of one-way and two-way coupling. The solvers were successfully implemented using the OpenFOAM finite volume method framework, and parallelized for distributed calculation on high-performance computing facilities.

The partially decoupled model was used to study the impact of a wide range of operational and material parameters on quantitative and qualitative aspects of the behaviour of the dust field. Dust particle properties in particular were seen to have a significant effect on the distribution of the dust through the arc region, as well as the quantity of dust bypassed relative to that captured by the bath surface. Location of the feed inlet was also seen to have a substantial impact on the dust circulation, with inlets located close to the electrode resulting in substantially improved capture of dust by the molten bath surface.

A brief examination of the effect of the dust on the arc via full coupling between the dust concentration field and the energy and momentum equations demonstrated that the presence of dust in the plasma gas could cause increased arc instability. Higher dust concentrations were seen to exacerbate this effect in the model results.

Much work remains to be conducted in this area.

Extension of the coupling models to include separate temperature and velocity fields for the dust would improve the accuracy of the calculations. Inclusion of some form of empirical turbulence modelling (either Reynolds-averaged or large eddy simulation variants) would be valuable for scaling the simulations to larger, industrial-scale furnaces. Combining the DC plasma arc and dust models with a free-surface multiphase flow model to more accurately calculate the shape of the bath surface below the arc would also be of interest, in order to examine the role that the dynamics of the arc cavity plays in dust dispersal and capture. Experimental study by injecting dust into the vicinity of an operating arc would also be of great value in proving or disproving the hypotheses arising from the model results.

Acknowledgements
This work is published by permission of Mintek. Interactions with personnel and facilities at the CSIR/Meraka Institute Center for High Performance Computing and the CSIR Aeronautics Systems Group during the development phase of this work were useful and are greatly appreciated.

References


SEW-EURODRIVE carries a large local stock holding of this robust product – with its unique modular production concept. Developed as one of the most powerful industrial gear units, this unit is available in finely stepped sizes covering torque ranges of up to 475kNm. A large number of pre-defined accessories offer a high degree of flexibility for adapting to a broad range of applications.

Why is this good news for you? Higher accuracy, faster turnaround times and more flexibility on your individual designs are available to you locally! Units are assembled and serviced locally, offering you less downtime and more productivity.

This is what we call Drive 360° - Seeing the big picture

SEW-EURODRIVE - Driving the world.

Tel: +27 11 248-7000
Web: www.sew.co.za
A finite difference model of the iron ore sinter process

by J. Muller*, T.L. de Vries*, B.A. Dippenaar*, and J.C. Vreugdenburg*

Synopsis

Iron ore fines are agglomerated to produce sinter, which is an important feed material for blast furnaces worldwide. A model of the iron ore sintering process has been developed with the objective of being representative of the sinter pot test, the standard laboratory process in which the behaviour of specific sinter feed mixtures is evaluated. The model aims to predict sinter quality, including chemical quality and physical strength, as well as key sinter process performance parameters such as production rate and fuel consumption rate. The model uses the finite difference method (FDM) to solve heat and mass distributions within the sinter pot over the height and time dimensions. This model can further be used for establishing empirical relationships between modelled parameters and measured sinter properties. Inputs into the model include the feed material physical properties, chemical compositions, and boundary conditions. Sub-models describe relationships between applied pressure differential and gas flow rate through the bed of granulated fine ore particles, combustion of carbonaceous material, calcination of fluxes, evaporation and condensation of water, and melting and solidification. The model was applied to typical sinter test conditions to illustrate the results predicted, and to test sensitivities to parameters such as feed void fraction, feed coke percentage, and the fraction of combustion heat transferred to the gas phase. A model validation and improvement study should follow, ensuring sinter test results are free from experimental errors by conducting repeated tests.

Keywords

iron ore sintering, finite difference method, coke combustion, calcination, evaporation and condensation, melting and solidification, sinter strength.

Introduction

Blast furnaces are predominantly used for ironmaking, with more than 90% of the world’s clean iron units produced in these processes (Kogel et al., 2006). High-grade lump iron ore, high-grade ore fines, and concentrates from lower grade ores are utilized as feed to blast furnaces. These ore fines are agglomerated typically through sintering or pelletization to improve the blast furnace burden permeability, reducing the coke consumption rate and improving reduction rate. Sinter is used as blast furnace feed at percentages of up to 90%, and contributes to reduced operating costs (Kogel et al., 2006).

Research and development for the sintering process on the laboratory or pilot scale is typically conducted by means of a sinter pot test. The VIU (Value In Use) team at Kumba Iron Ore routinely uses sinter pot tests to evaluate new sinter raw materials, primarily in terms of production rate, coke consumption, and product sinter physical properties. Optimum sinter blends can be investigated as well as the impact of changes in sinter blends on the sintering performance and sinter quality, providing information for marketing of the iron ore. As such, the VIU sinter pot test equipment is in high demand.

Sinter pot tests are time-consuming, thus the turnaround time can be slow. The tests are also very costly. For these reasons, it is clear that a modelling tool that could predict the key outcomes of sinter tests with a reasonable level of accuracy would be a valuable tool for assessing the performance of sinter blends in the initial phases of a project. It is not expected that the model could replace the pot test, but that it would complement the pot test work and possibly reduce the number of actual tests required. This paper discusses the work done to date towards this goal.

The sinter pot test

The continuous industrial sintering belt process is approximated by using a batch ‘pot’ test in which the material contained in the stationary sinter pot passes through the same process stages as it would on a sinter belt. Sinter pot test measurements are used as basis for the validation of one-dimensional (1D) models (Patisson et al., 1991; Zhou et al., 2012a). The sinter pot test is illustrated in Figure 1.

The procedure for the sinter pot test is as follows. After the equipment is prepared, the raw material blend is manually weighed and fed into the test pot via a high-intensity mixer and a granulation drum. Once the pot has been...
A finite difference model of the iron ore sinter process

Filled, key settings, including the ignition time and temperature and the pressure drop set-points of the various stages, are entered on the sinter control system via the SCADA interface. Typically, the applied pressure differential below the pot is pressure-controlled rather than flow rate controlled, and the material in the pot is ignited using LP gas.

After ignition, the temperature is manually controlled by the operators by regulating the gas flow rate. The ignition stage ends automatically after the prescribed time has elapsed and the process proceeds to the sintering stage. The end of sintering is defined as the time at which the peak exhaust gas temperature is measured, indicating that the flame front has travelled all the way through the sinter cake. An optional cooling cycle may be included after this, where cold air continues to be drawn through the sinter cake. However, this is used only occasionally.

After sintering is completed, the sinter cake is removed from the pot using an overhead crane. The cake then proceeds to physical and metallurgical testing. This starts with a set of drop tests followed by a drum breakdown procedure; after which the sample is screened to determine the size distribution of the final sinter. The FeO content of the sample is measured by titration. Additional tests are conducted: a tumble index (TI) test as per ISO 3271, a reducibility index (RI) test as per ISO 4695 and ISO 7215, and a reduction disintegration (RDI) test as per ISO 4696-1 and 4696-2. If required, REAS (Reduktion, Erweichung, und Abschmelzen – meaning reduction, softening, and melting) tests are also carried out to determine the softening and melting characteristics of the sinter.

The performance of a sinter in the pot test is defined by several measures, including productivity, fuel rate, and the strength and reactivity of the sinter as defined by the physical and metallurgical tests listed above. In order for a sinter model to be useful to VIU, it ultimately needs to be able to predict all of these parameters with a reasonable degree of accuracy. To validate the sinter model, sinter pot tests would typically be conducted in which additional thermocouples are mounted in the pot at various depths so that the measured temperature profiles in the sinter cake can be recorded and compared with those predicted by the model. Thermocouples are typically inserted at depths of 100 mm, 230 mm, and 420 mm, measured from the top of the sinter pot.

Sinter modelling

General principles

The sinter pot test can be simulated by modelling the mass and heat transfer phenomena occurring within the sinter bed over time as the boundary conditions change. Chemical reactions, heat transfer, and physical transformation can be modelled, and the temperature profiles, chemical compositions, gas flow velocities, etc. predicted. Physical strength parameters of the final sinter can be estimated through correlations with some of these predicted variables. Previous researchers have developed several such models describing iron ore sintering with various degrees of complexity (Dash et al., 1974; Thurlby, 1988; Patisson et al., 1991; Clixby and Young, 1992; Yang et al., 2004; Majumder et al., 2009). More recently, Zhou et al. (2012a) also reported on the development of such a model, and evaluated such work currently available in the literature (Zhou et al., 2012b).

The sinter pot test itself is a transient problem with heat and mass transfer occurring in all three dimensions, but predominantly in the height dimension as the flame front travels downwards through the sinter bed. It is therefore typical to assume variations over the area of the sinter pot to be negligible, and to model the sintering process using a transient 1D approach as illustrated in Figure 2 (Zhou et al., 2012b).

The transformation of a 1D section of solid material (control volume) from the sinter bed (Figure 2a), which includes a returned (recycled) sinter fines layer at the bottom (grit), is modelled over time. Gas flow in the model is from the top to bottom of this ‘control volume’. The solids temperature and chemical composition profiles are modelled over time, as well as the change in temperature and chemical composition of the gas flowing from top to bottom. The variable profiles along the sinter bed height (e.g. solids temperature, shown in Figure 2a) are combined for all of the time steps simulated to produce an illustration such as Figure 2b, showing solids temperature. This illustrates the complete
sinter process from start to finish, representative of the 'control volume' of material, which moves at the speed of the sinter strand. Variables may also be illustrated over time and at a specific depth, for example, the solids temperature as shown in Figure 2c.

**Model inputs**

Initial and boundary conditions that have to be specified as inputs to the model include the following:

- **Individual feed materials specification** (e.g. each ore, flux, fuel, etc.): amount of each constituent in feed mixture (recipe), chemical composition, particle size distribution, physical properties (density, porosity)

- **Granulated feed material** (mixed feed to the sinter pot) and bottom grit layer specification: particle size, void fraction, and sphericity

- **Sinter product requirement**: basicity (CaO/SiO₂), and percentages of FeO, MgO, and SiO₂ (optional)

- **Sinter process/boundary conditions**: bed and grit layer heights, ignition duration, ignition gas temperature, chemical composition, pressure at top of bed, and applied pressure differential below bed (for first and second ignition stages, and then normal sintering)

- **Simulation controls**: number of height elements, duration of time step, simulation maximum time, iterative calculation controls, sub-model control parameters, and results derivation parameters (e.g. sintering time defining temperature).

The amounts of ores, fuels, return fines, burnt lime, and moisture are specified in terms of the ratios making up the granulated feed. The amounts of other fluxes (dolomite, silica, lime) are determined for the feed blend prior to model calculation, in order to achieve the required sinter product basicity (CaO/SiO₂) and percentages of MgO and SiO₂.

The model allows for the void fraction to be estimated from the JPU (Japanese Permeability Unit) that is often measured for the granulated sinter feed material in separate test work. The actual pressure drop over the standardized JPU test sample is calculated using Equation [1] (Lwamba and Garbers-Craig, 2008). The material void fraction is iteratively determined using the Ergun equation (Equation [2]) with the other physical material properties of the sinter feed.

\[
JPU = \frac{V}{A \left( \frac{H}{\Delta P} \right)^{0.6}}
\]

where

\[ \Delta P \]: pressure drop (mm H₂O)
\[ H \]: height (mm)
\[ V \]: air flow rate (Nm³.min⁻¹)
\[ A \]: area (m²).

**Model solution**

The finite difference method (FDM) has been used to solve transient mass and energy conservation equations. The modelling approach followed and software algorithm are in principle the same as those described in more detail elsewhere (Majumder et al., 2009). An overview of the method is provided here, but for brevity the conservation and other model equations are not been repeated, unless they were different to those used in previous studies (Majumder et al., 2009) or of specific importance as stated later.

The control volume (illustrated in Figure 2a) is divided into collections of elements representing gas and solid separately. Variables defined for each element include temperature, chemical composition, reaction rates, etc. For
A finite difference model of the iron ore sinter process

solid elements, the liquid fraction is also defined as a variable, whereas for the gaseous elements, variables are also defined for velocity and pressure.

The combustion of carbonaceous material with oxygen from the air drawn in at the top of the sinter bed primarily determines the amount of heat generated, causing melting of solid phases and therefore forming the basis of the sintering process. The air flow velocity is controlled by the applied pressure differential at the bottom of the sinter bed, and is influenced by the physical properties of the solids, and by heat transfer and the chemical reactions occurring. The model iteratively determines the mass flow rate of gas drawn into the sinter at each simulated time step (Figure 2a). The gas-solid heat and mass transfer is calculated in each element by moving from the top to bottom and using sub-models to describe physical phenomena. After calculation of all the sub-models and the resulting heat and mass transfer between the solids and gas, the pressure drop is calculated over each solid material element, and the air flow rate into the bed adjusted until the total calculated pressure drop converges to that specified as the model input. The pressure drop is calculated as follows using the Ergun equation (Majumder et al., 2009):

\[ \frac{\Delta p}{L} = 150 \left(\frac{1 - \varepsilon}{\varepsilon}ight) \left(\frac{1 - 0.17\varepsilon}{0.17\varepsilon}ight) + 1.75 \left(\frac{1 - \varepsilon}{0.17\varepsilon}\right) \rho g \varepsilon U^2 \]

where

- \( \Delta p \): pressure drop (Pa)
- \( L \): height (mm)
- \( \mu_g \): gas viscosity (Pa.s)
- \( \varepsilon \): bed void fraction
- \( \phi \): particle sphericity
- \( d_p \): mean particle diameter (m)
- \( U \): gas velocity (m.s\(^{-1}\))
- \( \rho \): gas density (kg.m\(^{-3}\)).

Another important aspect of the energy balance calculated in each element is the assumptions made with respect to the heat of reaction from chemical reactions. Solid and/or gas phase species react with each other to yield products that are also in either the solid and/or gas phase (e.g. Equation [3]). In the energy balance of the model, the heat of reaction is split between the enthalpies of the solids and gas products (Yang et al., 2004). For each of the chemical reactions identified, a fraction \( y \) is specified as the fraction of the heat distributed to the gas, with the balance to the solids. For the chemical reactions the model parameters are defined as important model inputs that greatly affect the predicted temperature profiles – \( y_{calc} \) dolomite calcination; \( y_{comb} \) coke combustion; \( y_{evap} \) evaporation; \( y_{cond} \) condensation.

\[ \lambda(s) + B(g) \rightarrow C(s) + D(g) \]

Sub-models

Sub-models are formulated to model the gas-solid heat transfer and mass transfer due predominantly to chemical reactions as the gas enters at the top and moves through the sinter bed. Convective heat transfer between gas and solids is modelled only, with conduction and radiation excluded for simplification. Depending on the nature of the chemical reactions, heat is generated or consumed by the chemical reactions and distributed between the resulting gas and solid phases. Chemical reactions are modelled for water evaporation and condensation, dolomite calcination, coke combustion, and melting and solidification of all materials, including Fe raw materials. The physical transformation of the solids (e.g. bed shrinkage) and its effect on the bed permeability is not modelled here due to the unavailability of experimental data. The details on each of these sub-models is implemented in the sinter model and are provided below.

Convective heat transfer

Heat transfer between the downward-moving gas and solids particles in the sinter bed occurs mostly by means of forced convection. Heat transfer rate is calculated in each finite element from the relevant solids and gas temperatures, and a modelled heat transfer coefficient, \( h_{gs} \), using the model reported by Majumder et al. (2009) and Pattison et al. (1991):

\[ h_{gs} = \frac{\varnothing v_g \rho_g C_{pg}}{6(1 - \varepsilon_b) \xi} \]

where

- \( h_{gs} \): convective solid-gas heat transfer coefficient (W.m\(^{-2}\).K\(^{-1}\))
- \( \varnothing \): particle sphericity
- \( v_g \): gas viscosity (Pa.s)
- \( \rho_g \): gas density (kg.m\(^{-3}\))
- \( C_{pg} \): gas specific heat (J.kg\(^{-1}\).K\(^{-1}\))
- \( \varepsilon_b \): bed void fraction
- \( \xi \): channelling length factor.

Water evaporation and condensation

Water evaporates from the wet granulated feed in the warmer areas of the sinter bed around where the flame front progresses downwards through the sinter bed. As the gas flows through the unsintered bed, it carries this water vapour downwards into cooler areas of the bed below the flame front, where condensation becomes possible.

The rates at which evaporation (drying) or condensation occur in each solids element are estimated using the model reported by Pattison et al. (1990). Firstly, the mass transfer rate in the gas boundary layer is modelled as a function of the gas temperature and pressure, the gas-solid heat transfer coefficient, and the logarithmic mean of the actual and saturated molar fractions of moisture in the gas phase (Pattison et al., 1990):

\[ k = \frac{h T_g}{3.155 P \sqrt{\left(1 - 0.24 X_m\right) \left(1 + \frac{X_m}{P}\right) \left(1 - X_m\right)}} \]

where

- \( k \): boundary gas layer mass transfer rate (m.s\(^{-1}\))
- \( h \): heat transfer coefficient (W.m\(^{-2}\).K\(^{-1}\))
- \( T_g \): gas temperature (K)
- \( P \): absolute gas pressure (Pa)
- \( X_m \): logarithmic mean of actual and saturated molar fraction moisture in vapour.

The rate of moisture transfer is then calculated, depending on the actual moisture partial pressure (Pattison et al., 1990):

\[ r_a = \frac{a_g k}{R T_g \left(p_{H_2O}^at - p_{H_2O}^t\right)} \]
A finite difference model of the iron ore sinter process

where

- \( r_w \): rate of moisture transfer (mol.m\(^{-3}\).s\(^{-1}\))
- \( \alpha \): boundary specific area (m\(^2\).m\(^{-3}\))
- \( k \): boundary gas layer mass transfer rate (m.s\(^{-1}\))
- \( R \): ideal gas law constant (J.mol\(^{-1}\).K\(^{-1}\))
- \( T_s \): gas temperature (K)
- \( p_{H_2O}^\text{sat} \): H\(_2\)O saturation partial pressure in gas (kPa)
- \( p_{H_2O} \): actual H\(_2\)O partial pressure in gas (kPa)

This is then used to model the rate of moisture transfer between the gas and solids phases, and is also dependent on the specific area of the solids, and the actual and saturation H\(_2\)O partial pressures in the gas phase. Condensation is modelled to occur at a constant rate, independent of the amount of moisture in the solids. Evaporation is modelled also to occur at a constant rate up to a critical moisture content, after which the rate decreases in the ratio, \( P(W_r) \) (Pattison et al., 1990):

\[
P(W_r) = 1 - (1 - W_r) (1 - 1.796W_r + 1.0593W_r^2)
\]

where \( W_r \) is the ratio of the actual moisture content to the critical moisture content. A critical moisture content of 5% was used here (as per Majumder et al., 2009).

**Limestone and dolomite calcination**

CaCO\(_3\) and MgCO\(_3\) are present in some of the sinter feed materials, typically as dolomite and lime. These species start to decompose at a certain temperature in the sintering process, enriching the gas with CO\(_2\). The decomposition rates are modelled for CaCO\(_3\) and MgCO\(_3\) in each solids finite element using simple rate equations as functions of the solids temperature at that point (as per Thurlby, 1988):

\[
k_{ls} = 8.3 \times 10^{6} \exp\left(-\frac{18300}{T_s}\right)
\]

\[
k_{ms} = 0.25 \times 10^{6} \exp\left(-\frac{11200}{T_s}\right)
\]

where

- \( k_{ls} \): calcination rate constant of CaCO\(_3\) (1.s\(^{-1}\))
- \( k_{ms} \): calcination rate constant of MgCO\(_3\) (1.s\(^{-1}\))
- \( T_s \): solids temperature (K).

**Coke combustion**

Coke (and possibly other carbonaceous materials) is added to the sinter feed mixture as the fuel source. The carbon reacts with oxygen to produce CO and CO\(_2\), generating the heat required to initiate melting of the solids and assimilation of the remaining particles. Sinter models reported in the literature apply different combustion models, which also consider the generation and further combustion of CO, as well as the Boudouard reaction whereby CO\(_2\) is converted back to CO. Here the combustion model by Gibb and Field has been applied (as per Mei et al., 2010). In this approach the above combustion reactions are combined as follows, where the degree of oxidation is represented by the parameter \( \phi \):

\[
\theta C + O_2 \rightarrow 2(\theta - 1)CO + (2 - \theta)CO_2
\]

The parameter \( \phi \) is modelled as a function of temperature (Equation [5]). At lower temperatures CO\(_2\) is predicted as the main product, while at higher temperatures (from around 1000K) mostly CO is predicted as the Boudouard reaction is predominant (Zhou, 2012a).

\[
\frac{2(\theta - 1)}{2 - \theta} = A_s \exp\left(-\frac{T_s}{T_p}\right)
\]

where \( T_p \) is the particulate (solids) temperature (K), and \( A_s \) and \( T_s \) are model parameters with values of 2500K and 6240K respectively, as suggested by Mei et al. (2010).

The overall coke combustion rate is determined by the diffusion rate of oxygen to the reaction surface and by the carbon reaction rate. The oxygen diffusion rate equation is solved analytically to yield the coke combustion reaction rate equation in terms of the external oxygen diffusion rate, the surface reaction rate, and the rate of internal diffusion and surface reaction (Mei et al., 2010). The coke combustion rate is calculated with the Gibb model as a function of the parameter \( \phi \) and other parameters, including the coke particle physical properties, far field oxygen concentration, external and internal gas diffusion coefficients, and the particle (solids) temperature. The following set of equations, as reported by Mei et al. (2010), describes the model:

\[
\frac{dm_c}{dt} = -\frac{3\theta M_c C_w}{(1 - \epsilon) M_{O_2} \rho_c} (k_1^{-1} + (k_2 + k_3)^{-1})^{-1}
\]

\[
k_1 = \frac{D_{O_2\/N_2} R_p}{R_p^2}
\]

\[
k_2 = (1 - \epsilon) \frac{k_c}{R_p}
\]

\[
k_3 = \frac{k_c (\beta \coth \beta - 1)}{\beta \alpha}
\]

\[
\beta = R_p \left( \frac{k_c}{D_{O_2\/C\/E} \epsilon \alpha} \right)
\]

where

- \( m_c \): rate of carbon mass, \( m_c \) decrease (kg.s\(^{-1}\))
- \( \phi \): oxidation mechanism parameter, molar ratio of C to O\(_2\) atoms reacting
- \( \epsilon \): coke particle void fraction
- \( M_c \): carbon molar mass (kg.kmol\(^{-1}\))
- \( M_{O_2} \): oxygen molar mass (kg.kmol\(^{-1}\))
- \( C_w \): far field oxygen (O\(_2\)) concentration in the bulk gas (kg.m\(^{-3}\))
- \( \rho_c \): coke solid density (kg.m\(^{-3}\))
- \( k_1 \): rate of external diffusion (1.s\(^{-1}\))
- \( k_2 \): rate of surface reaction (1.s\(^{-1}\))
- \( k_3 \): rate of internal diffusion and surface reaction (1.s\(^{-1}\))
- \( D_{O_2\/N_2} \): external diffusion coefficient of O\(_2\) through N\(_2\) (m\(^2\).s\(^{-1}\))
- \( D_{O_2\/C\/E} \): internal diffusion coefficient of oxygen through coke particles (m\(^2\).s\(^{-1}\))
- \( R_p \): average coke particle radius (m)
**A finite difference model of the iron ore sinter process**

\[ k_c : \text{carbon oxygen rate (1.s}^{-1}) \]

\[ A_c : \text{carbon oxidation rate equation pre-exponential factor, 14.m}^{-1}s^{-1} \]

\[ T_c : \text{carbon oxidation rate equation constant, 21 580K} \]

\[ T_p : \text{coke particle temperature (solid temperature) (K)} \]

\[ \beta : \text{reaction parameter} \]

\[ a : \text{coke particle volume to internal surface ratio (m}^2.m}^{-2} \)

The diffusivities used above are calculated as follows as functions of the gas temperature, \( T_g \). The external diffusion coefficient of \( O_2 \) through \( N_2 \) (Majumder et al., 2009):

\[ D_{O_2/N_2} = 0.435 \times 10^{-5} \left( \frac{T_g}{298.15} \right)^{1.5} \left( \frac{0.29}{0.41} \right) \]

The internal diffusion coefficient of \( O_2 \) through coke particles (Dash et al., 1974):

\[ D_{O_2,C} = 1.8 \times 10^{-5} \left( \frac{T_g}{273} \right)^{1.5} \]

**Melting and solidification**

Melting and solidification are two of the most important phenomena in sintering since they enable particle assimilation and directly affect the physical properties of the sinter product. When the fines reach a certain temperature the primary melt forms, with its properties being a function of the temperature achieved and its chemical composition (Debrincat et al., 2004). The primary melt chemical composition is in turn influenced by the gradual assimilation of different individual particles into the melt, and subsequently also the bonding phases formed during solidification and the properties of the sinter product, e.g. sinter strength and reducibility (Debrincat et al., 2004).

This complex process of melting and solidification is simplified firstly by not specifically modelling the rate at which it occurs, based on the implicit assumption that heat transfer is rate limiting (modelled separately). A method by Zhou et al. (2012a) is used here to estimate the fraction melted as a function of the solids temperature and chemical composition of the fines fraction:

\[ \beta = \left( \frac{T_s - T_{sol}}{T_{liq} - T_{sol}} \right)^a \]

where \( \beta \) is the mass fraction of melted material, \( T_s \) is the solids temperature, \( T_{sol} \) is the solids temperature of around 1100°C, and \( T_{liq} \) is the liquidus temperature of the -1 mm fines fraction of around 1400°C (Zhou et al., 2012a). The value for the phase change factor, \( a \), depends on factors such the type of iron ore, particle size, ore porosity, and solids chemical composition (Zhou et al., 2012a). Due to these complexities, a value of 1 has been assumed for \( a \), similar to that used by Patterson et al. (1991) for estimating the fraction melted during solidification.

For each solids element, the fraction melting or solidifying is derived from the above relationship for that melted in the current and previous time steps. The heat of melting or solidification is derived and included in the energy balance of each element. An average of 0.254 MJ.kg\(^{-1}\) is used as the latent heat of melting, and 0.117 MJ.kg\(^{-1}\) for the latent heat of solidification. These values are the averages derived from other sources, as reported by Zhou et al. (2012a).

**Model outputs**

The model produces several outputs, which can be used to evaluate overall performance of the sinter mix and predicted sinter product properties with regard to the inputs specified, or to analyse the interrelated phenomena occurring in the sinter bed in order to make process improvements. In future, it may be possible to correlate some calculated model variables with some measured sinter properties, and these relationships may then be included in the model.

The model variables available for each element include:

- **Solids variables**: temperature, and chemical composition (wt.%)
- **Gas variables**: temperature, pressure, chemical composition (vol.%), velocity, and inlet mass flow rate
- **Reaction rates**: evaporation/condensation, limestone and dolomite calcination, and coke combustion reaction rates
- **Other parameters**: heat transfer coefficient, fraction melted and solidified, enclosed area above 200°C and 1100°C (as described in Zhou et al., 2012a).

Some of the more important model results calculated (before or after the simulation) are:

- **Bed void fraction**: calculated from the granulated feed material JPU Prior to the simulation, to be used then as a model input
- **Coke consumption rate**: coke usage rate calculated as the specified mass of coke feed divided by the calculated mass of sinter produced, with units of kg.t\(^{-1}\) sinter
- **Sinter product mass and chemical composition**: calculated from the feed material mixture specification, subtracting ignition loss components (e.g. carbon and carbonates)

### Table I

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Units</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Feed burnt lime</td>
<td>wt.% (wet)</td>
<td>3.0</td>
</tr>
<tr>
<td>Feed total return fines</td>
<td>wt.% (wet)</td>
<td>26</td>
</tr>
<tr>
<td>Feed total coke</td>
<td>wt.% (wet)</td>
<td>4.2</td>
</tr>
<tr>
<td>Feed moisture</td>
<td>wt.% (wet)</td>
<td>6.0</td>
</tr>
<tr>
<td>Sinter basicity target</td>
<td>wt.%</td>
<td>2.0</td>
</tr>
<tr>
<td>Sinter FeO target</td>
<td>wt.%</td>
<td>6.0</td>
</tr>
<tr>
<td>Sinter MgO target</td>
<td>wt.%</td>
<td>1.8</td>
</tr>
<tr>
<td>Sinter SiO2 target</td>
<td>wt.%</td>
<td>5.5</td>
</tr>
<tr>
<td>Sinter bed height</td>
<td>m</td>
<td>0.5</td>
</tr>
<tr>
<td>Grt height</td>
<td>m</td>
<td>0.25</td>
</tr>
<tr>
<td>Sinter bed diameter</td>
<td>m</td>
<td>0.3</td>
</tr>
<tr>
<td>Granulated feed bulk density</td>
<td>kg.m(^{-3})</td>
<td>2000</td>
</tr>
<tr>
<td>Feed void fraction</td>
<td></td>
<td>0.3</td>
</tr>
<tr>
<td>Feed particle diameter</td>
<td>m</td>
<td>0.004</td>
</tr>
<tr>
<td>Feed particle density</td>
<td></td>
<td>0.6</td>
</tr>
<tr>
<td>Sinter bed JPU</td>
<td></td>
<td>31.3</td>
</tr>
<tr>
<td>Combustion heat fraction to gas, (Y_{comb} )</td>
<td></td>
<td>0</td>
</tr>
<tr>
<td>Calcination heat fraction to gas, (Y_{calc} )</td>
<td></td>
<td>0</td>
</tr>
<tr>
<td>Evaporation heat fraction to gas, (Y_{evap} )</td>
<td></td>
<td>0</td>
</tr>
<tr>
<td>Condensation heat fraction to gas, (Y_{cond} )</td>
<td></td>
<td>0</td>
</tr>
<tr>
<td>Sinter bed suction pressure</td>
<td>mm (H_2O)</td>
<td>1010</td>
</tr>
<tr>
<td>Ignition temperature</td>
<td>°C</td>
<td>1098</td>
</tr>
</tbody>
</table>
A finite difference model of the iron ore sinter process

Table II
Iron-bearing feed material composition

<table>
<thead>
<tr>
<th>Species</th>
<th>wt.%</th>
</tr>
</thead>
<tbody>
<tr>
<td>FeO(s)</td>
<td>2.12</td>
</tr>
<tr>
<td>Fe₂O₃(s)</td>
<td>86.96</td>
</tr>
<tr>
<td>P(s)</td>
<td>0.044</td>
</tr>
<tr>
<td>S(s)</td>
<td>0.014</td>
</tr>
<tr>
<td>K₂O(s)</td>
<td>0.23</td>
</tr>
<tr>
<td>Na₂O(s)</td>
<td>0.048</td>
</tr>
<tr>
<td>CaO(s)</td>
<td>0.46</td>
</tr>
<tr>
<td>MgO(s)</td>
<td>0.22</td>
</tr>
<tr>
<td>Al₂O₃(s)</td>
<td>1.16</td>
</tr>
<tr>
<td>SiO₂(s)</td>
<td>5.03</td>
</tr>
</tbody>
</table>

➤ Sintering time: indicative of the speed with which the flame front travels through the bed and the sintering rate. Calculated as the time until the bottom of the bed cools to a specified temperature (e.g. 150°C)
➤ Burn-through times: similar to the sintering time, but calculated as the time to reach the maximum temperature below the sinter bed
➤ Production rate: rate of sinter produced calculated using the predicted mass of sinter produced and sintering time, typically units of t.m⁻² per 24 h

➤ Variable averages: variables (from the above list) averaged over the height of the sinter bed at the end of the simulation.

Results

Typical sinter pot test

The sinter model was configured to represent typical sinter test conditions to illustrate the results that could be generated. The most important model input parameters with typical values are summarized in Table I. In Table II the chemical composition of the iron-bearing feed material is provided. The sinter feed void fraction has been specified as 0.3 (Table I), similar to what was estimated for the specified feed JPU of 31.3, particle size of 0.004 m, and sphericity of 0.8 using the method described earlier and shown as a result parameter in Table III.

The model, predicted results are summarized in Table III. Together with the typical sinter performance parameters, the enclosed areas calculated above 1100°C are reported at different depths and on average over the sinter bed, which could be correlated to physical strengths measured of sinters produced in the test work.

Figure 3 illustrates the solids temperatures predicted by the model at depths of 100, 230, and 420 mm. This shows that the sinter bed temperatures increase sharply to over 1200°C, when melting starts to consume energy from the combustion reactions. As the coke is consumed, temperature decreases and the melted material solidifies.

Model sensitivities

Prior to conducting test work for model validation, the model (as defined in the previous section) was used to evaluate the sensitivities of certain model parameters. This evaluation was performed to provide guidance for subsequent experimental planning, model validation, and model improvements.

The void fraction of the sinter feed material could be derived from the solid and bulk densities, correlations with particle size, or from the actual JPUs as described earlier. These methods are likely to result in different values, and the bed void fraction is expected to change during sintering. The model was therefore used to estimate the sensitivity to void fraction by changing the baseline value of 0.3 by 10% in both directions. The temperature profiles predicted at a bed depth of 230 mm in Figure 4 show significant variations, with the times at which peak temperature is reached differing by

Table III
Model result parameter values

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Units</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Specific mass sinter produced</td>
<td>kg.t⁻¹ feed</td>
<td>895.3</td>
</tr>
<tr>
<td>Feed void fraction – estimated from JPU</td>
<td></td>
<td>0.30</td>
</tr>
<tr>
<td>Sintering time</td>
<td>min</td>
<td>25.7</td>
</tr>
<tr>
<td>Burn-through time</td>
<td>min</td>
<td>23.2</td>
</tr>
<tr>
<td>Burn-through rate</td>
<td>mm.min⁻¹</td>
<td>21.6</td>
</tr>
<tr>
<td>Production rate</td>
<td>t.m⁻² per 24 h</td>
<td>37.5</td>
</tr>
<tr>
<td>Coke consumption rate</td>
<td>kg.t⁻¹ sinter</td>
<td>69.1</td>
</tr>
<tr>
<td>Sinter yield</td>
<td>wt.%</td>
<td>87.3</td>
</tr>
<tr>
<td>Enclosed area over 1100°C – 100 mm depth</td>
<td>min. °C</td>
<td>33.9</td>
</tr>
<tr>
<td>Enclosed area over 1100°C – 230 mm depth</td>
<td>min. °C</td>
<td>109.9</td>
</tr>
<tr>
<td>Enclosed area over 1100°C – 420 mm depth</td>
<td>min. °C</td>
<td>250.5</td>
</tr>
<tr>
<td>Enclosed area over 1100°C – av.</td>
<td>min. °C</td>
<td>130.5</td>
</tr>
</tbody>
</table>

Figure 3 – Sinter bed temperatures predicted at 100, 230, and 420 mm depths
A finite difference model of the iron ore sinter process

Figure 4 – Predicted temperature at 230 mm bed depth for feed void fractions of 0.27, 0.3, and 0.33

Figure 5 – Predicted productivity as a function of the feed void fraction

Figure 6 – Predicted temperature at 230 mm bed depth for fractions of combustion heat to gas of 0, 0.25, 0.5, 0.75, and 1

Figure 7 – Predicted productivity as a function of the combustion heat fraction to gas

Figure 8 – Predicted temperature at 230 mm bed depth for feed total coke percentages of 3.8, 4.2, and 4.6%

Figure 9 – Predicted productivity as a function of the feed total coke percentage
A finite difference model of the iron ore sintering process

around 100 seconds. Figure 5 shows that the production rate decreases significantly for a lower void fraction, and increases for a higher void fraction.

Another model parameter with uncertainty is the fraction of combustion heat that is transferred to the gas. Figure 6 illustrates the change in temperature profiles predicted at a bed depth of 230 mm when this parameter is varied between 0 and 1. This shows that values larger than around 0.25 are less likely since the predicted peak temperatures are lower than what would normally be obtained in sinter test work. In further model development work the value of this parameter could be found for the best fit between predicted and measured temperatures. Figure 7 illustrates that the production rate increases slightly with higher fractions of combustion heat transferred to the gas.

The percentage of coke in the feed was also varied within ±10% of the baseline value of 4.2%. Figure 8 shows some variation in the predicted temperature profiles at a bed depth of 230 mm, with a generally wider profile and higher peak temperature predicted for higher percentages of coke as more heat is generated for a longer duration. This higher percentage coke results in slightly lower production rates as burn-through takes longer (Figure 9). This illustrates how the model could be used to find the optimum amount of coke in the feed, as well as the sensitivity to inaccuracies in the feed recipe.

Conclusions

A model of the iron ore sintering process was developed and solved using the finite difference method. The model was applied for typical sinter test conditions to illustrate results predicted, and sensitivities of certain parameters evaluated in preparation for test work to validate and further develop the model. Results were highly sensitive to the feed void fraction, which would therefore have to be determined with a high accuracy when performing test work for model validation. Further results indicated that the fraction of combustion heat transferred to the gas could possibly be varied between zero and around 0.25 to obtain an improved fit between predicted temperatures and those measured experimentally during model validation. The results also showed that wider temperature profiles with higher peak values are predicted for increased amounts of coke in the feed, resulting in lower production rates, which would be useful in applying the model to determine optimum coke feed rates. The outcomes of this study could be used to design a sinter test programme to validate and improve the sinter model. It is recommended that tests be repeated to confirm that the measurements are free from experimental errors prior to comparison with model results.

References


Leader in Insulating Brick and Chemical Plant Refractories

Adding value to the chemical and manufacturing industries of Southern Africa and the world.

Rietfontein is a manufacturer of insulating refractories and acid resistant brick and provides solutions to the chemical and manufacturing industries.

Our team of experienced refractory engineers, metallurgists and technicians can assist with problem identification, areas for improvement and training.

Verref is focused on building long term partnerships, adding value to our partner’s businesses from product specification to product disposal.

www.verrefshaped.co.za
Email: rietfontein@verrefshaped.co.za
Introduction

Rotary kilns are used for a range of mineral processing operations. Kilns range in size from 2–6 m in diameter and can be 50–225 m long with an operating mass of up to 3000 t. Two of the most common applications are cement production and sponge iron production. Hatch uses a proprietary one-dimensional kiln model to evaluate designs for clients (Haywood et al., 2009). This tool has been utilized for a variety of pyrometallurgical applications including ferrovanadium, nickel carbonate, nickel laterite, iron ore reduction, and spodumene (lithium) production.

This paper illustrates the application of numerical optimization techniques in combination with the kiln model in the interrogation of a generic iron ore reduction process. The fundamental modelling concepts are explained, followed by a description of the optimization approach. The results show how the combination of the two methods, with modern computing power, can generate a large number of viable design and operating candidates.

The FORTRAN model provides information on the solids and gas temperature evolution along the kiln, as well as a prediction of the reduction profile and off-gas composition. The bed profile and residence time from the Excel calculation form part of the input required by the FORTRAN program. The program allows comparison of results for a variety of geometric and operating conditions, including bed profiles, mass flow through the kiln, residence time, air profiles, ore and coal composition, and others parameters (a total of 108 input variables were defined for the example in this paper).

In the case of a generic iron ore reduction kiln (Figure 1), Table I provides an overview of the parameters (and ranges) that are considered.

The first part of the paper presents an overview of the kiln modelling method. The second part shows how the process is automated and combined with a numerical optimization scheme. The result is a powerful approach to kiln operational optimization. Illustrative examples are included for the case of iron ore reduction in a generic rotary kiln.

Rotary kiln model

Kiln modelling consists of two steps. Firstly, an Excel®-based calculation is used to determine the kiln bed profile and residence time based on specific operating conditions and the kiln configuration. This is followed by a calculation of the kiln operating characteristics with a FORTRAN program based on a one-dimensional model of the kiln’s mass and energy transfer.

The FORTRAN model provides information on the solids and gas temperature evolution along the kiln, as well as a prediction of the reduction profile and off-gas composition. The bed profile and residence time from the Excel calculation form part of the input required by the FORTRAN program. The program allows comparison of results for a variety of geometric and operating conditions, including bed profiles, mass flow through the kiln, residence time, air profiles, ore and coal composition, and others parameters (a total of 108 input variables were defined for the example in this paper).

In the case of a generic iron ore reduction kiln (Figure 1), Table I provides an overview of the parameters (and ranges) that are considered.

Synopsis

Rotary kilns are used for a variety of mineral processing operations. Hatch makes use of a kiln model developed from first principles to evaluate designs for its clients. This tool has been applied to a variety of pyrometallurgical applications, including ferrovanadium, nickel carbonate, nickel laterite, iron ore reduction, and spodumene (lithium) production.

This paper illustrates the application of numerical optimization techniques in combination with the kiln model in the interrogation of a generic iron ore reduction process. The fundamental modelling concepts are explained, followed by a description of the optimization approach. The results show how the combination of the two methods, with modern computing power, can generate a large number of viable design and operating candidates.

Keywords
direct reduction, DR process, rotary kiln, modelling, numerical optimization.
Modelling and optimization of a rotary kiln direct reduction process

Kiln residence time and fill level

Kiln residence time and fill level affect the progress of chemical reactions, as well as the maximum throughput for a rotary kiln. This is determined by (i) the maximum flow rate of the proposed burden through a kiln, and (ii) the residence time at temperatures that would allow sufficient reduction to take place.

A calculation method was developed that allows for the prediction of the bed profile and residence time in a rotary kiln. The method is based on the principle of granular movement in a kiln as described by Saeman (1951) and Scott et al. (2008). It assumes the kiln is operating in the rolling regime, the active layer has zero thickness, and the bed is locally flat. The experimental results provided by Scott et al. (2008) were used to validate the calculation method for different kiln and dam configurations. Figure 2 shows an example of the correlation between the model results and experimental data.

The method allows for the treatment of a number of geometrical parameters related to the kiln, including:

- Variations in kiln length, diameter, inclination, and rotation speed
- Straight or conical inlet and outlet configurations
- Stepped sections in the shell
- Conical or cylindrical-shaped dams inside the shell.

The limitations of the model include:

- No provision for density changes or material loss along the kiln length
- Lifters or chain sections cannot be considered
- The effects of gas velocity are neglected
- Transient effects in the bed are neglected.

The kiln under investigation does not have lifters or a chain section. Based on the good correspondence with experimental data, the other limitations in the model were not

<table>
<thead>
<tr>
<th>Table I</th>
</tr>
</thead>
</table>

| Model inputs used in the evaluation of the kiln performance |
|-----------------|---|
| **Design parameters** | Values |
| Kiln internal diameter | 4.34 m |
| Kiln length | 80 m |
| Kiln inclination | 1.5° |
| Solids angle of repose | 31° |
| **Operating parameters** | Range |
| Kiln rotational speed | 0.25–0.39 r/min |
| Bed residence time | 6–10 h |
| C/Fe ratio (based on reducible Fe) | 0.5–0.73 |
| Combined feed flow rate: cold feed | 48.8–54.0 t/h |
| Combined feed flow rate: hot feed | 60.6 t/h |
| Combined feed density range | 1895–2100 kg/m³ |
| Exit dam height | 0.7–1.0 m |
| Off-gas temperatures | 640–1210°C |

Figure 1 – Schematic of a rotary kiln

Figure 2 – Comparison of fill level calculation to experimental data
deemed to be critical for calculating bed profiles in the current investigation. Should greater accuracy be required, a discrete element method simulation of the bed flow would be recommended.

**One-dimensional kiln model**

The kiln model applied in this work was developed by Hatch over a number of years and has been used for several rotary kiln projects. It has its roots in a FORTRAN program that was developed by Venkateswaran (1978) to study the reduction of iron ore. The original software was used to model the operation of a 35 m pilot kiln at the Stelco company in Canada. A number of enhancements to the original Venkateswaran code have been added to increase the reliability and fidelity of the model. Examples of these enhancements include, but are not limited to:

- Incorporation of a bed level profile calculation along the length of the kiln
- Improved radiation modelling to account for view factors and gas participation at each axial node
- Extensive development of a comprehensive material database
- Inclusion of several additional chemical reaction schemes and kinetics (including ferrovanadium, nickel carbonate, nickel laterite, and spodumene)
- Code optimization to improve solution time by taking advantage of advances in modern compilers.

The kiln model is a one-dimensional finite-volume representation of the governing equations for mass and energy conservation, which are approximated by integration over discrete control volumes along the kiln length (i.e. axial slices). The solution of these discrete equations provides the local gas and solids temperatures and mass fluxes at each axial location along the kiln length.

In the bed phase the reactions may include the removal of moisture (free and bound) from the feed material, calcination of dolomite, as well as the Boudouard and Fe reduction reactions. The moisture removal from the bed is modelled with Arrhenius rate equations which describe the progress of the free and fixed moisture removal. The rate constants for moisture removal have been validated in earlier projects and were not modified for the presented calculations.

Where dolomite is included in the feed, it is assumed to consist of CaCO₃ only. Calcination occurs according to the reaction:

\[
\text{CaCO}_3(s) \rightarrow \text{CaO}(s) + \text{CO}_2(g)
\]

The reaction rate is effected through the use of an Arrhenius rate equation with constants as per previous applications of the model.

The Boudouard reaction is included as:

\[
\text{C}(s) + \text{CO}_2(g) \rightarrow 2\text{CO}(g)
\]

The reaction is modelled with a single step from haematite to metallic iron:

\[
\text{Fe}_2\text{O}_3 + 3\text{CO} \rightarrow 2\text{Fe} + 3\text{CO}_2
\]

The rates of the Boudouard and reduction reactions are prescribed by appropriate rate terms and determine the evolution of species concentrations and energy along the kiln.

The energy required for material heating, endothermic reactions, and heat losses is provided by the combustion of coal volatiles and char, combustion of CO gas from the Boudouard reaction, as well as a portion of the lance coal injected with ambient air at the discharge end of the kiln. The kiln model solves a comprehensive set of reaction equations using a Gibbs free energy minimization technique at the prevailing gas-phase temperature that yields realistic speciation of the reaction products. The effect of local conditions within the kiln, where thermal effects and chemical reactions in the bed may produce different species in the gas phase, is included in the model.

**Application of optimization**

The multivariable nature of a kiln operation can make it somewhat difficult for the analyst to find optimal combinations of operational or design variables through trial and error. Solution trends can be nonlinear and variables coupled in their influence on the solution. This calls for a more rigorous exploration of the design space through design of experiments and associated numerical techniques. Due to the need for the evaluation of a large number of design points, these techniques are well suited for use in combination with the one-dimensional kiln code, due to its relatively short solution time. LS-Opt software (LSTC) is used to coordinate the numerical optimization techniques and the automation of the solution evaluation.

One simple example of the use of this technique is the determination of the optimal distribution of secondary air introduced along the length of the kiln. The objective is to achieve a high level of metallization while respecting upper limits on the solids bed temperature. The aim of the design exploration is to find a secondary air distribution that achieves these objectives while keeping the off-gas volumes and temperatures low.

The optimization function formulated here is described as follows:

The objective: minimize \( f(x) \), the combined blow flow rate

Considering the variables:
- Blower rate on each of the 8 blowers, \([x_{1:8}]\)
- Coal feed rate, \([x_9]\)

Subject to inequality constraints:
- Max. bed temperature < 1250°C, \([g_{1}(x)]\)
- Max. outlet gas temperature < 850°C, \([g_{2}(x)]\)
- Metallization > 95%, \([g_{3}(x)]\)
- Outlet char > 10%/w, \([g_{4}(x)]\)

and side constraints:
- Blower rate on each of the 8 blowers: \(1000 < x_{1:8} < 7500\) Nm³/h, \([g_{5}(x)]\)
- Coal feed rate: \(5 < x_9 < 13\) t/h, \([g_{6}(x)]\)

**Results**

**Kiln model simulation**

The base case operation of the kiln was established by running the model with the design values for all operating parameters. The temperatures distributions in the bed, freeboard (gas), inner wall, and outer shell are shown in Figure 3 along the length of the kiln.

The feed material (bed) enters the kiln at ambient temperature and rapidly heats up due to the hot gas in the freeboard. At about 10 m into the kiln the volatiles are released from the coal, resulting in a local temperature spike.
Modelling and optimization of a rotary kiln direct reduction process

due to combustion of the volatiles in the freeboard. At the discharge end (80 m) the air injected into the kiln is rapidly heated by the burner. Despite the high freeboard temperatures, the shell temperature remains at about 200°C due to the refractory lining on the inside of the kiln.

The progress of mass transfer along the kiln length is presented in Figure 4. The metallization curve shows the start of metallization at around 20 m into the kiln, where the ore is reaching the required reduction temperatures. The exit value is 94% of the available Fe in the model (the model considers only 67% of the total Fe in the feed to take part in the reduction). In terms of the total Fe content in the feed, this represents a conversion of 65% Fe.

The curve representing the percentage bed carbon tracks the mass of the carbon in the bed in relation to the carbon added to the kiln feed inlet. The consumption of carbon by the Boudouard reaction follows the reduction reaction progress. It is clear that in the present case the bed is not depleted of carbon when the material reaches the kiln discharge.

Volatile release occurs rapidly from about 8 m into the kiln and is substantially completed at around the 25 m mark.

The gas composition in the freeboard is shown with gas partial pressure in Figure 5. The nitrogen partial pressure is plotted on the secondary y-axis and the rest of the components use the primary y-axis. The N2 and CO2 levels through the kiln are appreciably higher than other components.

Optimization

Considering the costs for a single experiment on a rotary kiln, minimizing the number of physical experiments is always an aim. Through formal design of experiments, this number is kept as low as possible and the most informative combination of the factors is chosen. In this example, five sequential design domains are considered, with sequential domain reduction. The space-filling point selection requires 83 design points per successive design space evaluation. The fully automated execution and evaluation of the 416 (83*5 + 1) design points is performed on a 12-core workstation within 70 minutes. Quadratic surrogate models are created for each set of results and provide a means to evaluate sensitivities and identify good candidate designs. A surrogate model, or metamodel (Gasevic et al., 2007), is a mathematical model that describes the behaviour of a system with respect to its variables. In the context of this paper, a quadratic metamodel is trained from the results of the individual analyses performed. This can be considered in much the same way as a quadratic trendline is fitted through data-points in a spreadsheet. Intuitively, the greater the number of analyses performed, the greater the confidence one has in the quality of the fit of the metamodel.

An illustration of this successive domain reduction (Stander et al., 2002) is shown in Figure 6, providing the results for the relationship between combined blower flow rate, outlet gas temperature, and maximum bed temperature. In the context of the confidence in the area of interest, the domain reduction ensures that sets of subsequent analyses are concentrated closer to the good candidate designs.

Results can be combined and good candidate designs shown within the complete cloud of results. Figure 7 provides point cloud plots for metallization with respect to combined blower flow, outlet gas temperature, and maximum bed temperature. The best candidate designs are highlighted to show their position in the cloud of results.
Figure 6 – 3D results plot showing successive domain reduction around the area of the good design candidates

Figure 7 – 2D results sets for metallization showing good candidate designs
Figure 8 shows key performance indicators of the best candidate designs relative to the base case design. The percentage improvement is shown in parentheses. Based on the spread of results, a preferred design can be selected as a trade-off between the best candidates. The base case design was based on a blower flow distribution applied from good kiln rules-of-thumb practice. Without the use of numerical optimization, this design is likely to have been the chosen operating condition imposed on the kiln. From the results, case 5.27 provides improvement of all key indicators with a significant drop in overall gas volume, exit gas temperature, and maximum bed temperature.

Conclusions
The direct reduction one-dimensional kiln model can be modified to accommodate any direct reduction process (not just iron ore), but will require physical test work and baseline calibration. This is usually part of the process for large projects, but was omitted here for brevity. The model allows evaluation of a comprehensive set of factors that may influence the kiln performance.

A certain class of problem lends itself to formal design of experiments and subsequent numerical optimization as an elegant means of design optimization. This paper illustrates how the one-dimensional kiln model can be coupled to the appropriate numerical tools to yield a powerful tool for kiln design and optimization. A significant number of design variables and design objectives (not an intuitive combination of input variables) can be evaluated in an automated fashion.

Key components of the success of the optimization are the accuracy of the kiln model and sensible interpretation of the model outputs. At Hatch the first component is addressed by working in close collaboration with clients during the model calibration phases to ensure model outputs are consistent with real experience. The second component is covered by ensuring that people with actual operating experience on the relevant equipment are included in the design team for the duration of the project.

References


Equipment selection based on the AHP and Yager’s method

by M. Yavuz*

Introduction

Multiple-criteria decision-making (MCDM) is one of the most considered branches of operation research. MCDM refers to making decisions that involve multiple, usually conflicting, criteria. The problems in MCDM are classified into two categories: multiple-attribute decision-making (MADM) and multiple-objective decision-making (MODM). However, the terms MADM and MCDM are often used to indicate the identical class of models and are confused in practice. Usually, MADM is used when the model cannot be stated in mathematical equations, otherwise MODM is used (Hwang and Yoon, 1980).

Decision-making is an important task in mining engineering projects, as in other engineering branches. Every mining engineer makes several decisions in daily mining applications. Most of the decisions made by mining engineers are completely instinctive, drawing from their past experience; therefore no decision-making method is applied.

Equipment selection is one of the most prominent problems in mining engineering. Mining engineers have to make difficult decisions during the equipment selection stage. As the decisions have a strong influence on the economic life of any mining scenario, they are considered as complex MADM problems. Therefore, the decision-maker can evaluate the subjective criteria concerning the problem of equipment selection. The decision-maker wishes to consider more than one objective criterion for the equipment selection stage. Among the number of alternatives, the most suitable equipment must be selected according to the objectives and alternatives. MADM applications can assist the decision-maker in achieving the optimal solution. In the mining industry, MADM methods can be applied for equipment selection because these methods include subjective and objective criteria that affect the selection among alternatives.

A review of the literature reveals that decision-making techniques have been used in different types of mining applications (Acaroglu, Feridunoglu, and Tumac, Alpay and Yavuz, 2007, 2009; Ataei, 2005; Ataei et al., 2008; Bitarafan and Ataei, 2004; Elevli and Demirci, 2004; Kazakidis, Mayer, and Scoble, 2004; Kesimal and Basci, 2002; Kluge and Malan, 2011; Namin et al., 2008; Yavuz, 2008; Yavuz and Alpay, 2008; Yavuz, Ipah, and Once, 2008).

In this paper, two different MADM methods – the analytic hierarchy process (AHP) and fuzzy multiple-attribute decision-making (FMADM) – are applied to select the loader for an open pit mine, and the solutions are compared.

Synopsis

One of the challenging problems for optimization in mining operations is to choose the best equipment among the alternatives. Equipment selection is an important task for mine management due to its operational cost, and is also an integral part of mine planning and design. Equipment selection is not a well-defined process because it involves the interaction of several subjective factors or criteria. Besides, decisions are often complicated and may even embody contradictions. Therefore, equipment selection is considered as a multi-criteria decision-making process, and suitable decision-making methods should be employed in this process. In this study, the loader selection for Aegean Lignite Colliery was made by using both the analytic hierarchy process and Yager’s method. Owing to the misusage of Yager’s method in the past, a new procedure is proposed in this paper for making proper decisions. It is highly recommended in this proposed method that criteria or alternatives should be grouped so as not to exceed the limitations of human performance (nine criteria/alternatives). The most appropriate solution for the loader selection was investigated by obeying this limitation for each method, and the results were compared. At the end of the decision-making process, a sensitivity analysis was applied for each method in order to see how a criterion affects the final decision. The advantages and disadvantages encountered during the application of each decision-making method are presented.

Keywords

AHP, Yager’s method, decision making, loader selection.

* Eskisehir Osmangazi University, Mining Engineering Department, Turkey.
Equipment selection based on the AHP and Yager’s method

Method
Equipment selection is important and difficult task to perform because of the need for handling many criteria simultaneously in the decision-making process. The number of criteria is important for arriving at the right decisions. A maximum of nine criteria can be handled in decision-making problems because of the general limitations of human performance (Saaty and Özdemir 2003). These limits are widely reported in the literature as the ‘memory span’, ‘attention span’, ‘central computing space’, and ‘channel capacity’ (Özdemir, 2005). If the pairwise comparison matrices are formed without considering these limits, then inconsistencies will likely occur. Even when the matrix is consistent, the matrix will likely not be valid. Therefore, the correct usage of the selected decision-making method is important to ensure the proper decisions. Because of the limitations mentioned in the AHP method, the total number of criteria for the Yager’s method should also be less than nine (Yavuz and Alpay, 2007).

AHP method
The AHP method developed by Saaty represents the interaction of multiple factors in complex unstructured situations (Triantaphyllou, 2000). This method is based on the pairwise comparison of components with respect to attributes and alternatives. A pairwise comparison matrix, \( A \), is constructed, where \( n \) is the number of elements to be compared. This method is applied for hierarchical problem structuring. The problem is divided into three levels: the problem statement, the object identification to solve the problem, and the selection of the evaluation criteria for each object. After structuring the hierarchy, the pairwise comparison matrix is constructed for each level in which a nominal discrete scale from 1 to 9 is used for the evaluation (Table I) (Saaty, 1980, 2000).

The next step is to determine the relative priorities of the criteria or the alternatives implied by this comparison. The relative priorities are determined using eigenvectors. For example, if the pair comparison matrix is \( A \), then the following can be written:

\[
(A - \lambda_{\text{max}} I) \times w = 0
\]  

[1]

To calculate the eigenvalue \( \lambda_{\text{max}} \) and eigenvector \( w = (w_1, w_2, ..., w_n) \), the weights can be estimated as relative priorities of the criteria or alternatives.

Because the comparison is based on a subjective evaluation, a consistency ratio is required to ensure the accuracy of the selection. The consistency index (\( CI \)) of the comparison matrix is computed as follows:

\[
CI = \frac{\lambda_{\text{max}} - n}{n - 1}
\]  

[2]

where \( \lambda_{\text{max}} \) is the maximal or principal eigenvalue, and \( n \) is the matrix size. The consistency ratio (\( CR \)) is calculated as:

\[
CR = \frac{CI}{RI}
\]  

[3]

where \( RI \) is the random consistency index. Random consistency indices are given in Table II (Saaty, 2000).

In general, a consistency ratio of 0.10 or less is considered acceptable. In practice, however, consistency ratios exceeding 0.10 occur frequently.

FMADM method
FMADM methods have been developed because of the lack of precision in assessing the relative importance of attributes and the performance ratings of alternatives with respect to an attribute. This imprecision may arise from a variety of sources, such as unquantifiable information, incomplete information, unobtainable information, and partial ignorance (Chen and Klein, 1997).

The main problem of a fuzzy MADM is to select/prioritize/rank a finite number of courses of action (or...
alternatives) by evaluating a group of predetermined criteria. Thus, to solve this problem, an evaluation procedure rating and ranking (in order of preference) of the set of alternatives must be constructed. The fuzzy MADM problem is described below:

1. A set of $m$ possible courses of action (referred to as alternatives):
   \[ A = \{A_1, A_2, \ldots, A_n, \ldots, A_m\} \]
2. A set of $n$ attributes (or criteria):
   \[ C = \{C_1, C_2, \ldots, C_j, \ldots, C_n\} \]
3. A performance rating of alternative $A_i$ with respect to attribute (or criterion) $C_j$ which is given by the $n \times m$ fuzzy decision matrix:
   \[ R = [R_{ij}]_{i=1, 2, \ldots, m; j=1, 2, \ldots, n} \]
   where $R_{ij}$ is a fuzzy set (or fuzzy number)
4. A set of $n$ fuzzy weights:
   \[ W = [W_j]_{j=1, 2, \ldots, n} \]
   where $W_j$ is also a fuzzy set (or fuzzy number) and denotes the importance of criterion $C_j$ in the evaluation of the alternatives (Chen and Klein, 1997).

Although a large number of FMA DM methods have been addressed in the literature, the focus of this paper is mainly on Yager’s method (Yager, 1978). This method is sufficiently general to address both multiple objectives and multiple attribute problems. Yager’s method follows the max-min method of Bellman and Zadeh (1970) with the improvement of the Saaty’s method, which considers the use of a reciprocal matrix to express the pairwise comparison criteria and the resulting eigenvector as subjective weights. The weighting procedure employs exponentials based on the definition of linguistic hedges as proposed by Zadeh (1973).

When describing MADM problems, only a single objective is considered, namely the selection of the best alternative from a set of alternatives. Yager’s method assumes the max-min principle approach. The fuzzy set decision is the intersection of all criteria: $\mu_D(A_i) = \min \{\mu_{C_1}(A_i), \mu_{C_2}(A_i), \ldots, \mu_{C_n}(A_i)\}$. For all $A_i \in A$, the optimal decision is yielded by $\mu_D(A^*) = \max \{\mu_D(A_i)\}$, where $A^*$ is the optimal decision.

The main difference in this approach compared with other approaches is that the importance of the criteria is represented as exponential scalars. This representation is based on the idea of linguistic hedges. The rationale behind using weights (or importance levels) as exponents is that the importance of a criterion increases, the exponent should increase, providing the minimum rule. Conversely, the less important a criterion, the smaller the weight. This process seems intuitive. Formally, this method can be written for $\alpha > 0$ (Bascetin and Kesim, 1999):

\[ \mu_D(A_i) = \min \{\mu_{C_1}(A_i)^{\alpha_1}, \mu_{C_2}(A_i)^{\alpha_2}, \ldots, \mu_{C_n}(A_i)^{\alpha_n}\} \]

### Modified Yager’s method

Because of the limitations mentioned in the ‘Methods’ section, the total number of criteria for Yager’s method should be less than nine (Yavuz and Alpay, 2007).

Therefore, a new procedure for Yager’s method is proposed in this paper for making proper decisions by taking into consideration the fact that the criteria or alternatives should be grouped so as not to exceed the limit of human performance (nine criteria/alternatives). In this method, the following steps should be applied to solve the problem in question with Yager’s method:

- Group the criteria into clusters with less than nine criteria
- Perform Saaty’s method for the main groups and calculate the weights for each group
- Perform Saaty’s method for all criteria in each group and calculate the weight of each criterion in the group
- Calculate the final weights of the criteria by multiplying the criteria weights with their own group weights.

### An application for loader selection

#### Description of the study site

In Turkey, coal production units controlled by the Etibank Company were transferred into Turkish Coal Enterprises (TKI) in 1957. In accordance with the Government’s general energy policy, TKI was assigned to produce lignite and other types of coal to satisfy the country’s coal demand, contribute to the economy, prepare and execute plans and programmes, determine application strategies, and to realize the strategies. The lignite reserves in Turkey total 13 billion tons, 4.5 billion tons of which are controlled by TKI. In total, 46 per cent of lignite production in Turkey is by TKI. TKI’s production depends on the requirements of the power generation companies and the demands from heating and industry. TKI produced 26.2 Mt of marketable coal in 2007 and 3.6 Mt through license. In 2007, TKI produced a picking of 268 million m3. In total, 79 per cent of the coal sold in 2007 (31.6 Mt) was supplied to the thermal plants operated by the electricity generation company.

Mining in the Aegean Lignite region has been ongoing since 1913. This region depended on the Western Lignite Colliery (GLI) from 1939 until 1978, and then operated under GLI until 1995. After 1995, the mines were operated by the Aegean Lignite Colliery (ELI). TKI received a regional directorate, operation directorate and was re-established as a legal entity in April 2004. After 2004, TKI established activities at the centre of the largest entity, Soma, and 90 miles away in Manisa (Figure 1).

In the township of Manisa, Soma has 610 Mt of lignite reserves with lower heating values between 2080–3150 kcal/kg. TKI holds these reserves, which are spread over 24.4 thousand hectares, and 71 per cent of these reserves are licensed to be exploited with underground operations by TKI.

![Figure 1 – The location of Soma and ELI](image-url)
Approximately half of the total sales of heating and industrial coal sold by TKI originate from this region. In addition, coal preparation and coal extraction plants are located in Soma. Opencast mining uses large-capacity excavators and heavy trucks. Underground mining is performed for the tender and the period of royalty; the annual production is 5.2 Mt. The total production of this establishment was 9.6 Mt in 2011.

**Defining the equipment selection process**

The AHP technique was used for wheel loader selection according to the criteria established by ELI. Selection criteria affecting the decision-making process should be considered in the AHP technique. The criteria used in this work to select the best alternative for a loader are the required technical features:

- Operating weight between 80 and 90 t
- Diesel engine with a net power exceeding 650 horsepower and suited for heavy working conditions
- Rated bucket capacity exceeding 12 cubic yards
- 45º discharge height exceeding 4 m
- Breakout force exceeding 60 000 kg
- Lifting capacity exceeding 17 500 kg
- Static tipping load exceeding 45 000 kg
- Articulating angle exceeding 30º
- Tyre protection chain should be available
- Rops-type operator cabin suited for all types of climate conditions
- L-5 class tubeless tyres resistant to wearing
- The machine should be equipped with a torque converter, full power shift, and four-wheel drive.

In addition to these technical features, the wheel loader should be able to operate in local conditions such as 1000 m of altitude, ambient temperatures of -25 to +40°C, and soil densities of 1.1 to 1.8 t/m³.

The criteria and sub-criteria were assessed by an expert team consisting of one mechanical engineer (the manager of the firm, with 10 years of experience in the mining industry) and two mining engineers with 20 years of experience in the mining industry. All decisions have a common hierarchical structure whereby options are evaluated against the various criteria to promote the ultimate decision objective. The problem of the loader selection was structured in a hierarchy of different levels constituting goals, criteria, sub-criteria, and alternatives (Figure 2).

**The AHP solution**

After structuring a hierarchy, the pairwise comparison matrix for each level is constructed. During the pairwise consideration, a nominal scale is used for the evaluation (Table I). As shown in Table III, each main criterion affecting the loader selection was compared, and the pairwise comparison matrix was constructed. The expert team performed these comparisons. The Economic Main criterion is the most important factor (priority 0.4714).

After constructing the pairwise comparison matrix for the main criteria, all subgroups of each main criterion should be compared (Tables IV, V, VI, and VII). The pairwise comparison matrices are constructed by comparing each loader alternative with each sub-criterion in all of the main criteria. The comparison matrix for the Capital Cost sub-criterion in the Economic Main criterion is given in Table VIII as an example, and the general evaluation of the alternatives is shown in Figure 2.
Equipment selection based on the AHP and Yager’s method

Economic Main criterion is given in Table IX. An identical procedure was applied for the other main criteria and associated sub-criteria.

The total priorities of the Economic Main criterion are calculated by summing the product of the relative priority of each sub-criterion and the eigenvalues considering the corresponding Economic Main criterion. The total priorities are calculated as the following: \((0.2329 \times 0.3882) + (0.4747 \times 0.2580) + (0.4668 \times 0.1612) + (0.2717 \times 0.1612) + (0.0861 \times 0.0314) = 0.3346 \) (Table IX).

The overall rating for each alternative is calculated by summing the product of the relative priority of each criterion and the alternatives considering the corresponding main criteria. For example, the overall rating of ‘Alternative A’ is calculated as the following: \((0.3346 \times 0.4714) + (0.1007 \times 0.1791) + (0.3723 \times 0.2533) + (0.3402 \times 0.0962) = 0.3028\). Similarly, the constructed final matrix is shown in Table X.

Because the comparison is based on a subjective evaluation, a consistency ratio (CR) should be calculated from Equation [3] to ensure the accuracy of the selection. From Tables III to VIII, the maximum eigenvalues \(\lambda_{\text{max}}\) are nearly the size of the matrix (in Table III, the size of the matrix is 4×4, and the mean value of \(\lambda_{\text{max}}\) is 4.1233), and

<table>
<thead>
<tr>
<th>Table IV</th>
<th>Pairwise comparison matrix for the Economy Main criterion with the associated sub-criteria</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>(C_{11})</td>
</tr>
<tr>
<td>----------</td>
<td>--------------</td>
</tr>
<tr>
<td>(C_{11})</td>
<td>1</td>
</tr>
<tr>
<td>(C_{12})</td>
<td>1/2</td>
</tr>
<tr>
<td>(C_{13})</td>
<td>3/4</td>
</tr>
<tr>
<td>(C_{14})</td>
<td>1/3</td>
</tr>
<tr>
<td>(C_{15})</td>
<td>1/6</td>
</tr>
</tbody>
</table>

\(\lambda_{\text{max}}=5.2500, \ CI=0.0625 \text{ and } CR=0.0558\%\), OK.

<table>
<thead>
<tr>
<th>Table V</th>
<th>Pairwise comparison matrix for the Operating criterion with the associated sub-criteria</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>(C_{21})</td>
</tr>
<tr>
<td>----------</td>
<td>--------------</td>
</tr>
<tr>
<td>(C_{21})</td>
<td>1</td>
</tr>
<tr>
<td>(C_{22})</td>
<td>1/2</td>
</tr>
<tr>
<td>(C_{23})</td>
<td>3</td>
</tr>
<tr>
<td>(C_{24})</td>
<td>4</td>
</tr>
</tbody>
</table>

\(\lambda_{\text{max}}=4.0206, \ CI=0.0069 \text{ and } CR=0.0076\%\), OK.

<table>
<thead>
<tr>
<th>Table VI</th>
<th>Pairwise comparison matrix for the Technical criterion with the associated sub-criteria</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>(C_{31})</td>
</tr>
<tr>
<td>----------</td>
<td>--------------</td>
</tr>
<tr>
<td>(C_{31})</td>
<td>1</td>
</tr>
<tr>
<td>(C_{32})</td>
<td>3</td>
</tr>
<tr>
<td>(C_{33})</td>
<td>1</td>
</tr>
<tr>
<td>(C_{34})</td>
<td>1/3</td>
</tr>
<tr>
<td>(C_{35})</td>
<td>1/2</td>
</tr>
<tr>
<td>(C_{36})</td>
<td>1</td>
</tr>
<tr>
<td>(C_{37})</td>
<td>1/3</td>
</tr>
</tbody>
</table>

\(\lambda_{\text{max}}=6.0776, \ CI=0.0111 \text{ and } CR=0.0079\%\), OK.

<table>
<thead>
<tr>
<th>Table VII</th>
<th>Pairwise comparison matrix for the Warranty criterion with the associated sub-criteria</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>(C_{41})</td>
</tr>
<tr>
<td>----------</td>
<td>--------------</td>
</tr>
<tr>
<td>(C_{41})</td>
<td>1</td>
</tr>
<tr>
<td>(C_{42})</td>
<td>3</td>
</tr>
<tr>
<td>(C_{43})</td>
<td>2</td>
</tr>
<tr>
<td>(C_{44})</td>
<td>3</td>
</tr>
</tbody>
</table>

\(\lambda_{\text{max}}=4.1880, \ CI=0.0627 \text{ and } CR=0.0698\%\), OK.

<table>
<thead>
<tr>
<th>Table VIII</th>
<th>Pairwise comparison matrix for the Capital Cost sub-criterion of the Economic Main criterion</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>(A)</td>
</tr>
<tr>
<td>----------</td>
<td>-------</td>
</tr>
<tr>
<td>(A)</td>
<td>1</td>
</tr>
<tr>
<td>(B)</td>
<td>3</td>
</tr>
<tr>
<td>(C)</td>
<td>1/2</td>
</tr>
<tr>
<td>(D)</td>
<td>1/3</td>
</tr>
</tbody>
</table>

\(\lambda_{\text{max}}=4.0511, \ CI=0.0170 \text{ and } CR=0.0189\%\), OK.

<table>
<thead>
<tr>
<th>Table IX</th>
<th>Total priorities of the Economic Main criterion</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>(C_{11})</td>
</tr>
<tr>
<td>----------</td>
<td>--------------</td>
</tr>
<tr>
<td>(A)</td>
<td>0.2329</td>
</tr>
<tr>
<td>(B)</td>
<td>0.5450</td>
</tr>
<tr>
<td>(C)</td>
<td>0.1385</td>
</tr>
<tr>
<td>(D)</td>
<td>0.0836</td>
</tr>
</tbody>
</table>

| Main     | 0.3082       | 0.2580       | 0.1612       | 0.1612       | 0.0314       |                 |

The Journal of The Southern African Institute of Mining and Metallurgy
VOLUME 115
MAY 2015
429
Equipment selection based on the AHP and Yager’s method

The CR values are less than 0.1 (in Table III, the mean CR value is 0.0457). These values are in the desired range. Therefore, this decision is selected without repeating the procedure.

Considering the overall results in Table X, Alternative A must be selected as the optimum loader selection to satisfy the goals and objectives of the TKI management because the priority of this alternative (0.3028) is the highest among all options.

For the loader selection, the proposed AHP model is unique in its identification of multiple attributes, minimal data requirement, and minimal time consumption. However, the most substantial general disadvantage of the AHP method is developing a large number of pairwise comparison matrices. Pairwise comparisons are often a stressful process for decision-makers.

The solution by Yager’s method

The calculation procedure by Yager’s method is identical to the AHP method both for the main criterion and sub-criteria in the problem in question.

The main criterion and sub-criteria weights are calculated identically as in the AHP method. The combined weights for the 21 sub-criteria are then calculated by multiplying each main criterion weight and each sub-criterion weight separately. The combined weights for each sub-criterion are given in Table XI.

The sum of the weights of this sub-criterion weight is 1. The calculated weight values for each sub-criterion are taken as membership functions of each sub-criteria. The exponential weights for each sub-criterion are given as follows:

\[ a_{11} = 0.1831, \ a_{12} = 0.1216, \ a_{13} = 0.0760, \ a_{14} = 0.0760, \ a_{15} = 0.0148 \]
\[ a_{21} = 0.0207, \ a_{22} = 0.0104, \ a_{23} = 0.0562, \ a_{24} = 0.0918 \]
\[ a_{31} = 0.0355, \ a_{32} = 0.0830 \]
\[ a_{41} = 0.0355, \ a_{42} = 0.0118, \ a_{43} = 0.0201, \ a_{44} = 0.0201, \ a_{45} = 0.0118 \]
\[ a_{51} = 0.0112, \ a_{52} = 0.0209, \ a_{53} = 0.0209, \ a_{54} = 0.0431 \]

The general weight values for each sub-criterion obtained from expert opinions are given as the ‘decision matrix’ in Table XII. The weights of each alternative for the sub-criteria are selected using fuzzy numbers ranging from 0 to 1.

By using membership levels of alternatives and the weight of criteria for each criterion, the following conclusions were reached using Equation [4]:

\[ \mu_D(\text{Alternative A}) = \min \{0.4 \times 0.1831, 0.2 \times 0.1216, 0.2 \times 0.0760, 0.4 \times 0.0760, 0.8 \times 0.0148, 0.4 \times 0.0207, 0.4 \times 0.0104, 0.4 \times 0.0562, 0.2 \times 0.0918, 0.4 \times 0.0355, 0.2 \times 0.0830, 0.4 \times 0.0201, 0.6 \times 0.0201, 0.4 \times 0.0201, 0.4 \times 0.0118, 0.2 \times 0.0112, 0.2 \times 0.0209, 0.4 \times 0.0431\} = 0.822. \]

\[ \mu_D(\text{Alternative B}) = \min \{0.2 \times 0.1831, 0.4 \times 0.1216, 0.6 \times 0.0760, 0.6 \times 0.0760, 0.6 \times 0.0148, 0.2 \times 0.0207, 0.6 \times 0.0104, 0.6 \times 0.0562, 0.4 \times 0.0918, 0.4 \times 0.0355, 0.2 \times 0.0830, 0.4 \times 0.0201, 0.6 \times 0.0201, 0.4 \times 0.0201, 0.4 \times 0.0118, 0.2 \times 0.0112, 0.2 \times 0.0209, 0.4 \times 0.0431\} = 0.822. \]

Table X

<table>
<thead>
<tr>
<th>Overall result/final matrix</th>
</tr>
</thead>
<tbody>
<tr>
<td>C1</td>
</tr>
<tr>
<td>-----</td>
</tr>
<tr>
<td>A</td>
</tr>
<tr>
<td>B</td>
</tr>
<tr>
<td>C</td>
</tr>
<tr>
<td>D</td>
</tr>
</tbody>
</table>

Table XI

<table>
<thead>
<tr>
<th>Main criteria</th>
<th>Sub–criteria</th>
<th>Weights</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Sub</td>
<td>Main</td>
</tr>
<tr>
<td>Economy (C1)</td>
<td>Capital cost (C11)</td>
<td>0.3882</td>
</tr>
<tr>
<td></td>
<td>Fuel cost/consumption (C12)</td>
<td>0.2580</td>
</tr>
<tr>
<td></td>
<td>Spare parts cost (C13)</td>
<td>0.1612</td>
</tr>
<tr>
<td></td>
<td>Auxiliary equipment cost (C14)</td>
<td>0.1612</td>
</tr>
<tr>
<td></td>
<td>Resale cost (C15)</td>
<td>0.0314</td>
</tr>
<tr>
<td>Operating (C2)</td>
<td>Material size (C21)</td>
<td>0.1158</td>
</tr>
<tr>
<td></td>
<td>Moisture (C22)</td>
<td>0.0579</td>
</tr>
<tr>
<td></td>
<td>Ground conditions (C23)</td>
<td>0.3138</td>
</tr>
<tr>
<td></td>
<td>Weather conditions (C24)</td>
<td>0.5125</td>
</tr>
<tr>
<td>Technical (C3)</td>
<td>Machine weights (C31)</td>
<td>0.1401</td>
</tr>
<tr>
<td></td>
<td>Flywheel power (C32)</td>
<td>0.3277</td>
</tr>
<tr>
<td></td>
<td>Bucket capacity (C33)</td>
<td>0.1401</td>
</tr>
<tr>
<td></td>
<td>Discharge height (C34)</td>
<td>0.0468</td>
</tr>
<tr>
<td></td>
<td>Breakout capacity (C35)</td>
<td>0.0792</td>
</tr>
<tr>
<td></td>
<td>Lifting capacity (C36)</td>
<td>0.0792</td>
</tr>
<tr>
<td></td>
<td>Static tipping load (C37)</td>
<td>0.1401</td>
</tr>
<tr>
<td></td>
<td>Articulating angle (C38)</td>
<td>0.0468</td>
</tr>
<tr>
<td>Warranty (C4)</td>
<td>Pleasure from the dealer (C41)</td>
<td>0.1169</td>
</tr>
<tr>
<td></td>
<td>Service conditions (C42)</td>
<td>0.2175</td>
</tr>
<tr>
<td></td>
<td>Spare parts providing (C43)</td>
<td>0.2175</td>
</tr>
<tr>
<td></td>
<td>Warranty (C44)</td>
<td>0.4481</td>
</tr>
<tr>
<td>TOTAL</td>
<td>4.0000</td>
<td>1.0000</td>
</tr>
</tbody>
</table>
Equipment selection based on the AHP and Yager’s method

Table XII

<table>
<thead>
<tr>
<th>Expert opinions</th>
<th>General weight values</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>A</td>
</tr>
<tr>
<td>C₁₁</td>
<td>0.4</td>
</tr>
<tr>
<td>C₁₂</td>
<td>0.2</td>
</tr>
<tr>
<td>C₁₃</td>
<td>0.2</td>
</tr>
<tr>
<td>C₁₄</td>
<td>0.4</td>
</tr>
<tr>
<td>C₁₅</td>
<td>0.8</td>
</tr>
<tr>
<td>C₂₁</td>
<td>0.4</td>
</tr>
<tr>
<td>C₂₂</td>
<td>0.4</td>
</tr>
<tr>
<td>C₂₃</td>
<td>0.2</td>
</tr>
<tr>
<td>C₂₄</td>
<td>0.2</td>
</tr>
<tr>
<td>C₁₁</td>
<td>0.4</td>
</tr>
<tr>
<td>C₁₂</td>
<td>0.2</td>
</tr>
<tr>
<td>C₁₃</td>
<td>0.4</td>
</tr>
<tr>
<td>C₁₄</td>
<td>0.4</td>
</tr>
<tr>
<td>C₁₅</td>
<td>0.6</td>
</tr>
<tr>
<td>C₁₆</td>
<td>0.2</td>
</tr>
<tr>
<td>C₁₇</td>
<td>0.2</td>
</tr>
<tr>
<td>C₁₈</td>
<td>0.2</td>
</tr>
<tr>
<td>C₁₉</td>
<td>0.2</td>
</tr>
<tr>
<td>C₂₀</td>
<td>0.4</td>
</tr>
<tr>
<td>C₂₁</td>
<td>0.2</td>
</tr>
<tr>
<td>C₂₂</td>
<td>0.2</td>
</tr>
</tbody>
</table>

The Minimum Values

0.822 0.745 0.656 0.707

0.80 0.0355, 0.60 0.0830, 0.20 0.0355, 0.20 0.0118, 0.20 0.0201, 0.40 0.0201, 0.40 0.0355, 0.60 0.0118, 0.40 0.0112, 0.60 0.0209, 0.80 0.0209, 0.20 0.0431 = 0.745.

μD(Alternative C) = min{0.60 0.1831, 0.80 0.1216, 0.80 0.0760, 0.20 0.0760, 0.40 0.0148, 0.80 0.0207, 0.20 0.0104, 0.80 0.0562, 0.80 0.0918, 0.60 0.0355, 0.40 0.0830, 0.60 0.0355, 0.60 0.0118, 0.40 0.0201, 0.80 0.0201, 0.80 0.0355, 0.10 0.0118, 0.60 0.0112, 0.60 0.0209, 0.40 0.0209, 0.60 0.0431} = 0.656.

μD(Alternative D) = min{0.80 0.1831, 0.60 0.1216, 0.40 0.0760, 0.80 0.0760, 0.20 0.0148, 0.60 0.0207, 0.20 0.0104, 0.40 0.0562, 0.60 0.0918, 0.150 0.0355, 0.80 0.0830, 0.60 0.0355, 0.40 0.0118, 0.80 0.0201, 0.60 0.0201, 0.60 0.0355, 0.40 0.0118, 0.80 0.0112, 0.20 0.0209, 0.60 0.0209, 0.80 0.0431} = 0.707.

Using the Bellman-Zadeh max-min rule, the structure of a decision is reached as follows:

μD(A) = [Alternative A / 0.822, Alternative B / 0.745, Alternative C / 0.656, Alternative D / 0.707]

The optimal solution is found as follows:

μD(A) = max{μD(Alternative A)} = 0.822. Therefore, ‘Alternative A’ is found to be the most appropriate wheel loader because it displays the highest membership function value.

Yager’s method consists of the identical order of operations as the AHP method, up to the calculation of all criterion weights. The most substantial difference between Yager’s method and the AHP is achieving the final solution using only one decision matrix. Therefore, Yager’s method involves fewer processing steps and fewer pairwise comparisons than the AHP method. Although not used in this study, decision-makers can include linguistic expressions in the decision-making process in the application of Yager’s method (Yavuz, 2008). This feature facilitates decision-making in a fuzzy environment.

Sensitivity analysis for each method

A sensitivity analysis must be performed to determine how the alternatives will change with the importance of the criteria. As the priority of one of the criteria increases, the priorities of the remaining criteria must decrease proportionately, and the global priorities of the alternatives must be recalculated. A sensitivity analysis can also be used to determine the most important or critical criterion by computing the absolute or percentage amount by which the weight of any criterion must be changed to cause a switch in the ranking of the top alternative or in any pair of alternatives (Triantaphyllou and Sánchez, 1997).

The values of the eigenvector for the main criterion in the pairwise comparison matrices simulated were increased or decreased for several scenarios in the AHP and FMADM methods. No change was noted in the judgment evaluations in the final priority ranking when the eigenvector value of each criterion increased/decreased up to 44 per cent in the AHP method (Figure 3). Therefore, ‘Alternative A’ can always be selected as the most convenient alternative for the decision-making process, and ‘Alternative B’, ‘Alternative C’, and ‘Alternative D’ sequentially followed in the final priorities. From the sensitivity analysis, the final result of the proposed AHP model is mainly sensitive to decreases in the Technical Main criterion.

However, the final decision found by the proposed FMADM model was compared with the simulated scenarios in Figure 4. When the priority of the all criteria increased or decreased by 50 per cent, the present decision does not change. Therefore, ‘Alternative A’ can always be selected as the most convenient alternative for the decision-making process, and ‘Alternative B’, ‘Alternative C’, and ‘Alternative D’ sequentially followed in the final priorities. From the
Equipment selection based on the AHP and Yager’s method

In the sensitivity analysis, by increasing or decreasing the values of the eigenvector of the main criterion, the variability limit is calculated as 61 per cent. After this limit, the Warranty Main criterion takes a negative value, increasing the Economic Main criterion. As previously mentioned, the AHP model is mainly sensitive to decreases in the Technical Main criterion, and the FMADM model is mainly sensitive to increases in the Economic Main criterion. Figure 5 and Figure 6 show respectively multiple runs of the sensitivity analysis for every 5 per cent change of the AHP and FMADM models according to its most sensitive criterion. These figures also indicate the accuracy of the applied decision-making process in both methods.

Conclusions

Mining engineers frequently have to select an optimum option among alternatives related to the mining operation. Each mining engineer might make precise decisions in all mining operations, and the decision-maker must use a suitable technique to make proper decisions. A number of techniques are available for solving different types of decision problems. In this study, the AHP and Yager’s methods, which are two similar MADM techniques, are used to solve an equipment selection problem.
Equipment selection based on the AHP and Yager’s method

References


THE DANIE KRIGE GEOSTATISTICAL CONFERENCE

GEOSTATISTICAL GEOVALUE REWARDS AND RETURNS FOR SPATIAL MODELLING

Crown Plaza, Johannesburg · 19–20 August 2015

THEME
The theme of the conference is ‘Geostatistical Geovalue—Rewards and Returns for Spatial Modelling’, a theme which emphasizes the improvement in, or addition to, value that spatial modelling can bring to the process of mine evaluation and mineral resource and reserve estimation. Spatial modelling of earth related data to estimate or enhance attributed value is the principle domain of geostatistics, the broad content of the Danie Krige Commemorative Volumes, and the focus of this conference.

OBJECTIVES
The conference provides authors who have recently published papers in the SAIMM’s Danie Krige Commemorative Volumes, a platform to present their research. In addition an invitation to geostatisticians, resource estimation practitioners, and those with an interest in geostatistics to present new papers for inclusion in the proceedings is now open. The conference will explore advances in technology and methodologies, and case studies demonstrating the application of geostatistics. It will cross the commodity boundaries, with applications presented from precious to base metals, and diamonds. This is a valuable opportunity to be involved in constructive dialogue and debate, and to keep abreast with the best practice in this specialist field.

WHO SHOULD ATTEND
The conference provides a platform for:
- local and international geostatisticians
- geologists
- engineers
- researchers
- software vendors
- mineral resource managers and practitioners, across the mining industry
- consultancy and academia, to present their work and contribute to the advancement of this field.

BACKGROUND
Geostatistics constitutes a globally accepted technical approach to mineral resource-reserve estimation and the basic toolkit for mine evaluation practitioners. Following the call for papers and the publication of the Danie Krige Commemorative Volumes, the SAIMM invites submission of papers for the Danie Krige Geostatistical Conference to be held in Johannesburg, South Africa, 19–20 August 2015.

CONFERENCE SUPPORTER

EXHIBITION/SPONSORSHIP
Sponsorship opportunities are available. Companies wishing to sponsor or exhibit should contact the Conference co-ordinator.

For further information contact:
Conference Co-ordinator, Yolanda Ramokgadi
SAIMM, P O Box 61127, Marshalltown 2107
Tel: +27 (0) 11 834-1273/7
E-mail: yolanda@saimm.co.za
Website: http://www.saimm.co.za
Introduction

During the preliminary design phases and feasibility study of a proposed vertical shaft, very little detailed information is available on the rock mass characteristics, in-situ rock stress, rock strengths, hydrological characteristics, and structural parameters can be determined using wireline logging of this borehole. In addition, a rock mass classification scheme is developed, based on published work, and in particular the Q-factor is adapted to assess the stability of raise-bored shafts. The ‘stick plot’ is introduced, which combines all geotechnical parameters applicable to the stability of a vertical shaft into a colour-coded format where cross-correlations can readily be made on a day-to-day basis during the shaft-sinking process.

Keywords
shaft-sinking, raise-boring, geophysical logging, geotechnical, Q-factor, stability.

Pre-sink shaft safety analysis using wireline geophysics
by N. Andersen*

Synopsis
During the preliminary design phases and feasibility study of a proposed vertical shaft, a vertical diamond drill-hole is normally drilled on the site. This paper outlines how rock mass characteristics, in-situ rock stress, rock strengths, and hydrological characteristics, and structural parameters can be determined using wireline logging of this borehole. In addition, a rock mass classification scheme is developed, based on published work, and in particular the Q-factor is adapted to assess the stability of raise-bored shafts. The ‘stick plot’ is introduced, which combines all geotechnical parameters applicable to the stability of a vertical shaft into a colour-coded format where cross-correlations can readily be made on a day-to-day basis during the shaft-sinking process.

Keywords
shaft-sinking, raise-boring, geophysical logging, geotechnical, Q-factor, stability.

* GeoScientific and Exploration Services, Irene.
© The Southern African Institute of Mining and Metallurgy, 2015. ISSN 2225-6253. Paper received May 2013 and revised paper received Jan. 2015

The deviated stick plot
The basis of the stick plot technique (Figure 1) is the use of Barton’s geotechnical parameters that have been adapted to a vertical tunnel using data derived from geophysical wireline logging. Each individual structure (jointing, fractures, bedding, breakout etc.) is identified in the core, and geologically and geotechnically described with exact depth, inclination, and azimuth. This geophysical data is used to support of horizontal tunnels and excavations, McCracken and Stacey (1989) adapted Barton’s Q-factor to the stability of raise-boring. Peck and Lee (2008) have also adapted the Bieniawski (1989) and McCracken and Stacey systems to assess the stability of raise-bored shafts.

The choice of the rock mass classification system used is very often client-dependent. However the ‘stick plot’ technique used here employs modified versions of Barton, as well as McCracken and Stacey, which have been enhanced with the use of wireline techniques and adjusted to various raise-bore diameters.

The purpose of the stick plot is to combine all geotechnical parameters applicable to the stability of a proposed shaft into an easily readable colour-coded format where cross-correlations can readily be made on a day-to-day basis during the shaft-sinking process. A detailed spreadsheet of all parameters is also provided for the use of the rock engineers.

The purpose of this paper is to introduce the stick plot method to the mining and shaft-sinking community as a viable alternative to the usually more esoteric methods of reporting, thus making the information readily accessible to all involved.
modify Barton’s, parameters such as joint set number ‘Jn’, joint water reduction factor ‘Jw’, and stress reduction factor ‘SRF’ for conditions in a vertical tunnel.

Both Bieniawski’s and McCracken and Stacey’s parameters are also adjusted using the more precise fracture/joint spacings and orientations derived from the geophysical data. The stick plot poster itself shows only the modified Barton (2002) data with an additional ‘sidewall stability index’. Barton’s (1974, 1976) Q-factor values for support/no support are plotted on the modified Barton bar chart to determine what length of the shaft would require support (Figures 2 and 3). A detailed spreadsheet is also supplied for the use of the rock engineers, showing all calculated parameters.

The parameters shown on the poster are for the day–to-day use of the shaft-sinkers, and include the following:

- Colour-coded modified Barton Q-factor normalized to shaft diameter
- Colour-coded sidewall stability index developed by Andersen Geological Consulting
- Stick plots showing dips of all structures subdivided into sets with the borehole deviation. There can be two or three sets, depending on the dominant structural sets
- Stereograms showing the orientation of the structural sets over 100 m intervals down the shaft. These diagrams show the orientation of sidewall bolting to achieve optimum anchoring
- Calculated UCS plotted in a barchart against the lithological log of the borehole
- Barton’s (1974, 1976) tunnel support charts showing the support/no support required using different Q-factor values (Figures 2 and 3).

**Details of modified parameters**

- RQD. Having accurately determined the positions of all the structures from the acoustic televiewer (ATV), geotechnical units are determined (where all structural spacings are similar) and the RQD is determined over these units, rather than at fixed intervals. The reason for this is that the RQD zone forms the basis of all of the derived parameters.

**Figure 1** – The shaft ‘stick plot’ showing the normalized Q-factor, the sidewall stability index, fracture orientations and calculated UCS superimposed on the geology

**Figure 2** – Barton’s (1974) tunnel support chart showing the the support/no support required for the shaft being evaluated
Pre-sink shaft safety analysis using wireline geophysics

► Jn (joint set number). Having measured the structural orientation, stereographic projections are plotted and Jn can then be accurately determined. The zone over which this calculation is done would depend on the dip of the structures and the diameter of the shaft.

► Jr and Ja. Each structure is identified on the ATV image so that its exact orientation and depth are known. Jr and Ja parameters are then directly linked to this position. Structural features such as brecciation and orientation of slickensides are also determined. This data then allows for a 'structural domain analysis' to be carried out on the data.

► Jw (joint water reduction factor). This factor is linked to the amount of water flowing from the fractures and also to the pressure. Before the water stratification in the borehole is disturbed by inducing water flow, a fluid conductivity log is run in the borehole. The size of the conductivity plume can then be related to the relative water ingress. This data is then interpreted along with physical observations of the fractures in the core, the televiewer classifications, the resistivity response given by the fractures, as well as the response of the full wave-form sonic tool. Following this, a wireline flow-meter can be used to determine the relative water ingress from fractures if a constant water flow is induced in the borehole from surface. This is often not possible as the fractures fill up and there is no flow of water.

► SRF (stress reduction factor). Weak zones intersecting the excavation which may cause loosening of the rock mass when the shaft is sunk. This is addressed by the sidewall stability index (SSI). Shear zones are clearly identified by the full-waveform sonic log, where P and S wave velocities of the sidewall are determined. The geotechnical log will also provide information about clay content and chemical alteration.

► Rock stress. The orientation of the principal stress can be determined if borehole breakout is visible on the televiewer imagery. The stress ratio can be determined from the geometry of the breakout. If the UCS is calculated over this zone then the value of the principal horizontal stress can be estimated.

► Rock strength. The elastic moduli can be calculated from the S- and -P-wave velocities derived from the full wave sonic geophysical log. These would include Young’s modulus, Poisson’s ratio, bulk modulus, and UCS. The UCS values are dynamic and are usually calibrated against laboratory measurements. The procedure is to take core samples from zones where there is a clean geophysical response, over a range of values and submit them for laboratory UCS determinations. A regression curve is calculated from the resulting data and the USC values are adjusted if necessary.

Sidewall stability index (SSI)

This is a parameter that was developed by Andersen Geological Consulting (2010) in order to quantify the stability of the sidewall of a raise bore. It is essentially an early warning system to alert the operators as to where sidewall conditions have deteriorated and sidewall collapse may occur. The index is not an absolute value, but is a probabilistic determination between ‘good’ and ‘very poor’ (Figure 4).

Barton (2002) takes the frictional component concept of his Q-factor further by referring to the fact that the ratio Jr/Ja closely resembles the dilatant or contractile coefficient of the friction for joints and filled discontinuities. The relative magnitude of \( \tan^{-1}(Jr/Ja) \) approximates the actual shear strength that might be expected of the various combinations of wall roughness and alteration products. Andersen (2010) combined this ratio with the true dip (from ATV) of the
Pre-sink shaft safety analysis using wireline geophysics

Figure 4 – The sidewall stability index. Matrix showing the calculation of the SSI based on angle of dip of the structure and shear strength derived from Barton’s Jr and Ja parameters

discontinuities and produced the sidewall stability index. This index relates to the stability of the sidewall, so dips were ranked from 60º to 90º, with a dip number of 2 being allocated to the category 60º to 65º, and 12 for the category 85º to 90º. Any dip less than 60º was given the value of unity. It was considered that dips of less than 60º were less likely to cause sidewall problems during raise-boring than steeper dips. The index has been expanded to include face stability, where fractures with low angles of dip are likely to drop out ahead of the raise bore. Here the dip number is inverted, with the flatter dips being given the higher dip numbers.

The stick plot technique has not been formally published, and was first used for the evaluation of several shafts at Impala Platinum over the period 2002 to 2004, followed by Lonmin Platinum in 2002, Western Platinum in 2003, at Lonmin Platinum’s Akanani Project in 2008, De Beers’ Venetia diamond mine in 2011, and Lonmin Platinum in 2013. The first public presentation of the technique was at a symposium of the SAIMM’s Bushveld Branch in 2004 (Andersen, 2004), followed by workshops given at Wits University, (Andersen, 2008, 2009). The concept of the sidewall stability index was first introduced at an SAIMM conference in 2010 (Andersen, 2010).

Summary of geotechnical results for the accompanying stick plot

The accompanying stick plot (Figure 1) is for the upper 400 m section of a 1 100 m borehole that was drilled for the evaluation of a shaft site. The graphic has been reduced in size for the purpose of publication.

The results below summarize the geotechnical evaluation of this borehole using the stick plot technique for the purpose of sinking a shaft.

Q-factor analysis

The Q-factor was calculated over the entire depth of the shaft borehole using intervals of RQD measurement. As stability varies with shaft diameter, an exercise was conducted to calculate the Q-factor for different diameters of raise bore. Shaft diameters of 6 m, 5 m, 4 m, and 3 m have been used. The Q-factor changes because the joint set number (Jn) becomes smaller as the shaft diameter decreases. The bar chart for the 6 m diameter shaft is shown in Figure 1. Superimposed onto this chart is the support/no support Q-factor value determined by Barton (1974, 1976). If Barton’s 1974 value of <1.4 is used, then for a 6 m diameter shaft, it is estimated that approximately 2% (16.1 m) of the length of the shaft would have to be supported. If the 1976 value of about 5 is used then approximately 35% (353.12 m) of the shaft would require support. The Q-factor values increase as the shaft diameter decreases. However, there is not a marked change as the fracture/joint dips are generally steeper than 60º.

The Q-factor analysis is used to estimate support/no support for horizontal tunnels, so it should be interpreted in conjunction with the sidewall stability index.

Sidewall stability index

The sidewall stability has been rated over the same intervals as the Q-factor and UCS and is shown as a bar chart on the stick plot. The sidewall stability is rated between medium and good down to a depth of 1006 m, after which there are some poor zones.

It is important to note that the SSI refers to the probability of the sidewall of the shaft collapsing during excavation. However, the normalized Q-factor indicates the blocky nature of the rock mass, which would be caused by the jointing and fracturing in the rock. In a horizontal tunnel this would relate directly to support required, whereas in a vertical shaft it indicates possible rock fragmentation after blasting. The SSI is a better indicator of sidewall stability.

In general the sidewall stability is reasonable but there are distinct zones where the dip of the fractures is greater than 60º and the fractures contain soft filling which could...
result in sidewall collapse. These zones are classified as poor on the SSI.

Below 860 m the jointing intensity increases and the Q-factor shows zones that are rated between fair and poor with some intervening sections being good. There is one very poor zone where there is a possibility of water inflow.

Overall trend of the structures
The banding and foliation are the most prominent structures present in the borehole. These have a mean strike direction of northwest to southeast, and dip dominantly to the southwest with a small component dipping to the northeast.

The jointing has been separately classified and is also seen to follow the dominant foliation direction, although the dips are steeper with an average of about 75°. A shallower dipping joint set is also present with a northwest to southeast strike and a dip to the southeast.

It was possible to classify dip, oblique, and strike slip faults. The orientations of the strike and oblique slip faults are sympathetic to the jointing. These faults dip at more than 70°. The dip slip faults form a conjugate set striking northwest-southeast and dipping at about 45° to both the northeast and southeast.

Sidewall bolting
A series of stereograms has been calculated over 100 m intervals down the length of the shaft. These show the mean dip and strike of the structures over each section. The purpose of these is to indicate the optimum direction for rockbolting, which is indicated by an arrow.

Groundwater intersections
The shaft will ‘make water’ from numerous joints from depths greater than 60 m, which is the current static water level. These are shown in column 6 as blue intervals. The driller’s log did not indicate any water intersections.

Rock strength analysis
The rock strength values, including UCS, Young’s modulus, and Poisson’s ratio, were calculated using the P- and S-wave velocities as determined from the full-waveform sonic measurements. The UCS values were overlaid onto the geological log on the stick plot and the other values are available as text files.

Conclusion
Barton’s Q-factor system (Barton et al., 1974) was initially developed to assess the design and support of horizontal tunnels and excavations. This system has been adapted for use in a vertical shaft, with structural information being derived from an acoustic televiewer (ATV) geophysical wireline log and Barton’s geotechnical parameters described directly from the borehole core at the depths indicated by the ATV log. A colour-coded bar chart is then constructed depicting Barton’s classification of rock mass quality between very poor and extremely good, based on RQD domains.

As the stability of the sidewall is very important in shaft sinking, a sidewall stability index (SSI) is introduced. This index is based on the dip of the structures (determined from the ATV) and the shear strength of the structure (J/Ja) determined from the geotechnical logging. Again, a colour-coded bar chart is derived, ranking the sidewall stability between good and very poor.

Zones of possible water inflow into the shaft excavation are indicated based on wireline fluid conductivity, differential temperature, and impeller measurements.

Stereographic projections are constructed based of structural measurements made by the ATV. Dominant joint sets are identified that could cause structural failure if their orientation is not taken into consideration when excavating shaft stations or developing shaft bottom orepass raises. These joint sets are shown as graphical projections.

Rock strength parameters are calculated from the wireline velocity and density measurements. The orientation of the principal horizontal stress is determined from the orientation of borehole breakout observed on the ATV image.

McCracken and Stacy’s (1989) maximum unsupported span, based on the geotechnical parameters, is also calculated but is not shown on the stick plot.

The ‘stick plot’ is designed as an easy-to-read graphic for the daily use of shaft sinkers to indicate rock conditions in advance of the sinking. A detailed report discussing the rock engineering parameters is also provided for the rock engineers.

References


Copper Cobalt Africa

In association with
The 8th Southern African Base Metals Conference
6–8 July 2015
Zambezi Sun Hotel, Victoria Falls
Livingstone, Zambia

Join us for the inaugural Copper Cobalt Africa Conference in the heart of Africa.

To be held at Victoria Falls, one of the Seven Natural Wonders of the World, this prestigious event will provide a unique forum for discussion, sharing of experience and knowledge, and networking for all those interested in the processing of copper and cobalt in an African context, in one of the world’s most spectacular settings.

The African Copper Belt has experienced a huge resurgence of activity in recent years following many years of political and economic instability. Today, a significant proportion of capital spending, project development, operational expansions, and metal value production in the Southern African mining industry are occurring in this region. The geology and mineralogy of the ores are significantly different from those in other major copper-producing regions of the world, often having very high grades as well as the presence of cobalt. Both mining and metallurgy present some unique challenges, not only in the technical arena, but also with respect to logistics and supply chain, human capital, community engagement, and legislative issues. This conference provides a platform for discussion of these topics, spanning the value chain from exploration, projects, through mining and processing.

For international participants, this conference offers an ideal opportunity to gain in-depth knowledge of and exposure to the Southern African base metals industry, and to better understand the various facets of mining and processing in this part of the world that both excite and frustrate the industry.

A limited number of places are available for post-conference tours to Kansanshi, the largest mine in Zambia, with 340 kt/y copper production and its soon-to-be-completed 300 kt/y smelter.

Jointly hosted by the mining and metallurgy technical committees of the Southern African Institute of Mining and Metallurgy (SAIMM), this conference aims to:

• Promote dialogue between the mining and metallurgical disciplines on common challenges facing the industry,
• Encourage participation and build capacity amongst young and emerging professionals from the Copper Belt region,
• Improve understanding of new and existing technologies, leading to safe and optimal resource utilisation.

The organising committee looks forward to your participation.
Hydraulic support instability mechanism and its control in a fully-mechanized steep coal seam working face with large mining height

by Y. Yuan*, S.H. Tu*, F.T. Wang*, X.G. Zhang* and B. Li*

Synopsis
Hydraulic support instability (HSI) is one of the most common causes of disasters in underground coal mining, posing a threat to the safety of mine workers and normal operation of the equipment. It is prone to occur in fully-mechanized mining faces with a large mining height (FMMLMH), especially when the dip angle of the coal seam is large. The key to controlling HSI is to deduce its mechanism and employ effective control techniques. This paper focuses on the analysis of HSI types, the key parameters and techniques to control HSI in FMMLMH, the establishment of a model of HSI in FMMLMH, and a multi-parameter sensitivity mechanical model of different HSI forms in the no. 7,19 longwall face in Xutuan Coal Mine, HuaiBei Mining Group, by using sensitivity analysis. The results show that HSI mainly presents in three forms: hydraulic support gliding (HSG), hydraulic support tilting (HST), and hydraulic support tail twisting (HSTT). The occurrence of the above three forms depends mainly on support anti-instability capability. In the no. 7,19 longwall face, HSG and HST are the main two forms of HSI. The dip angle of the working face and the friction coefficient between floor and hydraulic support are the sensitive parameters for HSG, while HST is strongly dependent on the dip angle of the working face and the friction coefficient between roof and hydraulic support. By the applications of measures such as the oblique layout of the working face, cutting the floor into a step pattern, moving the support under pressure, and raising the setting load, the support stability was controlled effectively.

Keywords
fully mechanized mining, mining height, hydraulic support instability, sensitivity analysis, sensitivity parameter, control technique.

Introduction
In 2013, coal production in China was 3680 Mt, accounting for more than one-third of the total world output. Production from thick seams accounts for 40–50% of national coal production. China is also the country with the highest incidence of mining disasters (Wu, Chen, and Long, 2012; Yuan, 2012). It is therefore essential to ensure mining safety in thick coal seams, especially concerning the prevention and control of hydraulic support instability (HSI), which poses a significant threat to the safety of mine workers and equipment (Tu, Yuan, and Yang, 2009). The most commonly used methods for mining thick coal seam (over 3.5 m), are fully mechanized mining with top coal caving (FMMTCC) and fully-mechanized mining with a large mining height (FMMLMH). Experience shows that recovery rate in FMMLMH is 10–15% higher than with FMMTCC. In recent years, with the development of mining equipment, FMMLMH technology has been widely used in thick coal seam mining. With its high recovery, FMMLMH has become a promising mining method for thick coal seams with a thickness less than 7.0 m (Ju and Xu, 2014).

However, due to the large mining height and intense induced ground pressure, HSI often occurs in FMMLMH, especially in the working faces of steeply dipping coal seams. The poor stability of hydraulic support and difficulty of HSI control are the chief obstacles to the widespread implementation of FMMLMH technology (Yuan et al., 2010). Therefore, the control of HSI has become one of the most vital techniques in FMMLMH (Yuan et al., 2010; He, Qian, and Liu, 1997). Figure 1 shows hydraulic support tilting (HST) in a FMMLMH working face with a dip angle of 15°. Considerable research has been done on these issues. He et al. (1997) reported measures to avoid HST when the roof was caving or the hydraulic support was moving. Gong and Jin (2001) studied the relationship between HST and its influencing factors. They claimed that dip angle, mining height, the height of centre of gravity of the hydraulic support, and sequence of hydraulic support movement can influence HST significantly. Hua and Wang (2008) studied HS stability of the inclined FMMLMH. Tu and Yuan investigated the HSI mechanism and its control in a FMMTCC face in a steeply inclined seam (Tu et al., 2008; Yuan et al., 2008). Wang analysed the stability and applicability of hydraulic support with a two-prop shield (Wang, 2009; Liu, 2006).
Hydraulic support instability mechanism

Most of the above studies focused on the role of factors such as mining height, dip angle, working resistance of hydraulic support, the hydraulic support gravitational height, and sequence of hydraulic support movement on HSI. There is still a lack of relevance and effectiveness in HSI control technology; it is difficult to make proper adjustments to control HSI effectively for a particular case. This paper establishes a HSI mechanical model for FMMLMH through the critical stability conditions under three main instability forms – hydraulic support gliding (HSG), hydraulic support tilting (HST), and hydraulic support tail twisting (HSTT). The sensitive parameters were obtained via multi-parameter sensitivity analysis of HSI. Based on the results, control measures were carried out to tackle the HSI problem, and satisfying results have been achieved in field applications.

Mechanical model of HSI

HSI mainly takes the forms of HSG, HST and HSTT in a FMMLMH working face (Yuan et al., 2008). In order to derive the following equations, we assume that the forces imposing on the hydraulic support from the overburden and the floor are both uniformly distributed and the hydraulic support has a sequence number from the top to the bottom, such as 1, 2, 3…, n where n is the total number of hydraulic supports in the working face).

Hydraulic support gliding

As shown in Figure 2, due to the combined influence of hydraulic support weight \( W \), the overburden resultant force \( P \), the floor resultant force \( R \), and the force between the adjacent support \( T_s \) and \( T_x \), the hydraulic support tends to glide along the floor.

In order to avoid HSG, the anti-gliding force, which can be calculated from Equation [1] (Gong and Jin, 2001; Yuan et al., 2008; Yuan, 2011), should be not less than the gliding force.

\[
T_s = Pf_1 \cos \alpha + (W + P)f_2 \cos \alpha \geq (W + P)\sin \alpha + T_x
\]  

where \( f_1 \) is the friction coefficient between roof and hydraulic support, \( f_2 \) is the friction coefficient between floor and hydraulic support, and \( \alpha \) is the dip angle of the working face.

Assuming \( n_h \) is the number of HSG, then the following situations apply:

1) If \( n_h=1 \) and \( T_s = T_x \), i.e. the number of HSG is one, then Equation [1] can be divided into two cases:

Case 1: the hydraulic support does not contact the roof, i.e. \( P=0 \), then Equation [1] can be simplified as \( f_2\tan\alpha \). That is, the condition of hydraulic support remaining stable under its own weight.

Case 2: the hydraulic support contacts the roof, i.e. \( P>0 \).

The critical angle of HSG \( \alpha_{th} \) can be obtained by Equation [1] as follows:

\[
\alpha_{th} = \arctan\left( f_2 + \frac{Pf_1}{P + W}\right)
\]  

In general, \( f_1 \) is affected by the structural integrity of the roof, and varies from 0.35 to 0.40; \( f_2 \) is affected by floor water, float coal, and period weighting pressure, and varies from 0.22 to 0.82 (Gong and Jin, 2001).

According to Equation [2], \( \alpha_{th} \) is proportional to \( P, f_1 \) and \( f_2 \); \( \alpha_{th} \) is inverse to \( W \).

2) If \( 1<n_h<n \) and \( T_s=T_x \), i.e. one HSG leads to the glide of adjacent supports, some supports in one certain area will glide. Assuming the first hydraulic support in the upper face glides, then \( T_s=0 \), and the induced force to the second hydraulic support can be calculated through Equation [3]:

\[
T_{hl(1-2)} = (W + P)\sin \alpha - [P\cos \alpha f_1 + (W + P)\cos \alpha f_2]
\]  

Similarly, the gliding force induced by \( n_h \) supports is:

\[
n_hT_{hl(1-2)} \leq T_s + k[\sin \alpha - \alpha] + (W f_2 \cos \alpha - \sin \alpha)
\]  

where \( T_{hl(1-2)} \) is the gliding force from the first hydraulic support to the second.

According to Equations [3] and [4], the support group tends to glide with increasing \( \alpha, n_h \) and decreasing \( k \).

3) For the case \( n_h=n \), as all of the supports glide, the smallest anti-gliding force to maintain stability of the support is \( n\alpha_{th(1-2)} \). This case occurs only rarely and is easy to control.

Hydraulic support tilting

With the existence of an inclination component of force along the coal seam, the point of resultant force deviates from the lower edge of the support, which is the reason for the support

Figure 1– HSG in a FMMLMH working face
Figure 2 – Model of HSG and HST
Hydraulic support instability mechanism

As shown in Figure 2, on the condition of the moment-limiting balance of torque, the point of reacting force is $O$. In order to avoid HST, the anti-tilting torque should no less than the tilting torque, and can be calculated from Equation [5] (Gong and Jin, 2001; Hua and Wang, 2008; Yuan et al., 2008; Yuan, 2011):

$$T_s - T_x = (P + W + WC) \sin \alpha + \left( P \frac{B}{2} + W \frac{B}{2} + P_f h \right) \cos \alpha \leq 0$$

where $h$ is the mining height, $B$ is the width of the HS base, and $C$ is the height of the centre of gravity of the hydraulic support.

Assuming the number of HSTs is $n_d$, then the following relationships can be derived.

(1) For the case $n_d=1$, $T_s = T_x$, i.e. the number of HSTs is unity, this circumstance can be divided into three conditions.

(a) The hydraulic support does not contact the roof, i.e. $P=0$. Equation [5] can be abbreviated as

$$\tan \alpha \leq \frac{B}{2C}$$

which is the condition for hydraulic support to keep in balance in the free state.

(b) The hydraulic support contacts the roof, i.e. $P>0$. The critical angle of HST $\alpha_{dl}$ can be derived from Equation [5] as follows:

$$\alpha_{dl} = \arctan \left[ \frac{B}{2C} \left( \frac{P + W}{2} + f_1 WC \right) \right]$$

According to Equation [6], the possibility of HST becomes smaller when the value of $\alpha_{dl}$ increases under the following conditions: $C$ decreases, $f_1$ or $B$ increases. There is an arc tangent function relationship between $1/h$ and $\alpha_{dl}$, and the suitable mining height decreases as $\alpha_{dl}$ increases. That is why the hydraulic support tends to tilt when mining height increases, even in coal seams with a low dip angle as shown in Figure 1.

(c) The hydraulic support tends to tilt when hydraulic support falls or moves or when the roof is caving or broken. The loading pressure $P$ then decreases, even to $P=0$. Then Equation [6] can be simplified as

$$\alpha_{dl} = \arctan \left( \frac{B}{2C} \right)$$

i.e. the value of $\alpha_{dl}$ depends mainly on

$$\frac{B}{2C}$$

(2) For the case $1<n_d<n$, $T_s \neq T_x$, assuming the first hydraulic support of the upper face end tilts, the pressure on the second hydraulic support $T_{dl(1-2)}$ can be calculated by Equation [7]:

$$T_{dl(1-2)} = P \left[ \sin \alpha - \frac{B}{2} + f_1 \cos \alpha \right] + \frac{W}{2h} \left( 2C \sin \alpha - B \cos \alpha \right)$$

Similarly, the pressure transferred from the $i$-th to the $i$-th hydraulic support is defined as $T_{dl(i-1)-i}$. Assuming there is a hydraulic support group formed by $j$ supports beneath the $i$-th hydraulic support, the stability of the hydraulic support group can be ensured through Equation [8]:

$$\left( T_{dl(i-1)-i} - T_i \right) h \leq \frac{B}{2} \left( P \frac{B}{2} + W \frac{B}{2} + P_f h \right) \cos \alpha - \left( P + W + WC \right) \sin \alpha$$

According to Equation [8], the hydraulic support becomes more stable with decreasing dip angle and increasing $i$ and $j$.

(3) For the case $n_d=n$, all the supports of the working face tilt. This situation is not tolerated in field production, and will not be discussed in this paper.

Hydraulic support tail twisting

The height of the caving zone is much larger in a FMMLMH working face. The impulse force due to the caving rock after hydraulic support moves will cause the tail part of the hydraulic support to twist. If the anti-twist capacity of the hydraulic support is not enough to resist the lateral force caused by the component force due to caving in a down-dip direction, the tail of the hydraulic support will rotate and cause the support to tilt. An increase in the dip angle of the working face will aggravate this phenomenon.

As shown in Figure 3, $L$ is the distance from the working line of the resultant force $P$ from the roof to the end part of the top beam; $L_d$ is the distance from the working line of the resultant force from the floor to the projection of the end part of top beam on the substructure; $D$ is the length of the tail beam; and $\theta$ is the rotation angle of the tail beam.

The weight of caving rock on the hydraulic support tail beam $G$ can be expressed as:

$$G = BH \gamma D \sin \theta$$

![Figure 3 – Mechanical model of the anti-twist analysis in the tail of the hydraulic support](image-url)
Hydraulic support instability mechanism

where \( H \) is the caving rock height, \((\text{metres})\) and \( \gamma \) is the average force per unit volume, \((\text{kN/m}^3)\).

The torque force of caving rock on the hydraulic support tail beam \( F_1 \) can be expressed as:

\[
F_1 = G f_3 \sin \alpha \sin \theta \tag{10}
\]

where \( f_3 \) is the friction coefficient between caving rock and hydraulic support tail beam.

The torque \( M_1 \) can be expressed as:

\[
M_1 = G \frac{D \sin \theta}{2} f_1 \sin \alpha \sin \theta \tag{11}
\]

The anti-twist force along the roof \( F_2 \) caused by \( P \) can be expressed as:

\[
F_2 = P f_1 \cos \alpha \tag{12}
\]

The torque force along the floor \( F_3 \) caused by \( R \) can be expressed as:

\[
F_3 = (P + W) f_1 \cos \alpha \tag{13}
\]

Then the anti-torque \( M_2 \) can be expressed as:

\[
M_2 = [(P + W) f_3 + P f_1] \cos \alpha \tag{14}
\]

In the case \( M_2 > M_1 \), hydraulic support remains stable, and the critical angle of hydraulic support tail tilting \( \alpha_0 \) can be expressed as:

\[
\alpha_0 = \arctan \left( \frac{2P f_1 f_3 + 2(P + W) L_d f_3}{B H D^2 f_1 \sin^3 \theta} \right) \tag{15}
\]

It is important to note that the above analysis depends on the axis being located in the midpoint of the top beam end. The axis position changes with the development of gliding. It may locate in the midpoint of the substructure end, and the analysis procedure is similar to the above.

According to Equation (15), the possibility of HSTT becomes smaller when the value of \( \alpha_0 \) increases under the conditions as follows: \( f_1 \), \( f_2 \), \( P \), \( W \), \( L \), or \( L_d \) increases, and \( B \), \( H \), \( f_2 \), \( D \), or \( \theta \) decreases.

Based on the above analysis, the instability of one support is the cause of the unstable support in the working face. Whether the HSI is controlled effectively depends on the relationship between the critical instability angle and the dip angle of the working face. To evaluate the HSI quantitatively, a stability factor \( K \) is included:

\[
K = \frac{\alpha_0}{\alpha} \tag{16}
\]

where \( \alpha_0 \) is the critical instability angle and \( \alpha \) is the dip angle of the working face. There are three possible scenarios, depending on the value of \( K \):

- \( K > 1 \), the hydraulic support is stable
- \( K = 1 \), the hydraulic support is in a critical balanced state
- \( K < 1 \), the hydraulic support is unstable.

The value of \( K \) is the least value of three parameters \( K_h \), \( K_d \), and \( K_n \), i.e.:

\[
K = \min(K_h, K_d, K_n) \tag{17}
\]

where \( K_h \), \( K_d \), and \( K_n \) are the coefficients of anti-glide, anti-tilting, and anti-tail twisting for the hydraulic support, respectively:

\[
K_h = \frac{\alpha_0}{\alpha} = \frac{\arctan(f_3 + \frac{P f_1}{P + W})}{\alpha} = \frac{P(f_1 + f_3) + W f_3}{(P + W) \tan \alpha} \tag{18}
\]

\[
K_d = \frac{\alpha_0}{\alpha} = \frac{\arctan(f_1 + \frac{(P + W) B - 2 f_3}{2(Ph + WC)})}{\alpha} \tag{19}
\]

\[
K_n = \frac{\alpha_0}{\alpha} = \frac{\arctan(\frac{2P f_1 L + 2(P + W)L_d f_3}{BHD^2 f_1 \sin^3 \theta})}{\alpha} \tag{20}
\]

According to Equations (17)–(20), there are many factors affecting the HSI, including \( \alpha_0 \), \( f_1 \), \( f_2 \), \( f_3 \), \( P \), \( W \), \( b \), \( D \), \( h \), \( L \), \( D \), and \( \theta \). It is a complex systematic problem to analyse the impact of the above factors on the HSI. Thus, it is necessary to conduct a quantitative analysis on the problem. Sensitivity analysis provides a new method of solving such a problem.

The sensitivity analysis method

The sensitivity analysis method (SAM) is a systemic analysis method focusing on the stability of a system (Zhang and Zhu, 1993; Zhu and Zhang, 1994; Hou et al., 2005).

Assuming that there is a system, the characteristic \( U \) is determined by factors in the number of \( m \), \( \beta_1 = \{\beta_1, \beta_2, \ldots, \beta_m\} \). The system characteristic is under the criterion state \( \beta = \{\beta_1, \beta_2, \ldots, \beta_m\} \). The definition of SAM is the trend and degree of deviation of \( U \) from \( U^* \), due to changes of each factor in its own possible range.

The first step of SAM is to establish a system model, i.e. forming a function relationship between the systematical characteristics and factors \( U = \{\beta_1, \beta_2, \ldots, \beta_m\} \). It is much better to define the function relationship with an analytic expression. For the complex system, numerical and diagrammatic methods are also appropriate to represent the function relationship. The establishment of the system model, conforming to the practical system to its greatest extent, is the key to the effective analysis of the parameter sensitivity.

It is necessary to provide a criterion parameter set, which is based on the specific questions. For example, the rock mass characteristics in a specific working face can be taken as a criterion parameter set to analyse the sensitivity of support stability to the given parameters. Sensitivity analysis can be conducted as the criterion parameter set has been defined. When the influence of parameter \( \beta_k \) on the characteristic \( U \) is analysed, the remaining parameters are taken as criterion parameters and remain constant, \( \beta_k \) varies in the possible range, and then \( U \) can be expressed:

\[
U = \phi(\beta_1, \beta_2, \ldots, \beta_k, \beta_1', \beta_2', \ldots, \beta_m') \tag{21}
\]
Hydraulic support instability mechanism

Table I
Main technical parameters of ZY11000/28/63 hydraulic support

<table>
<thead>
<tr>
<th>Item</th>
<th>Parameter</th>
<th>Item</th>
<th>Parameter</th>
</tr>
</thead>
<tbody>
<tr>
<td>Centre distance (m)</td>
<td>1.75</td>
<td>Supporting height (m)</td>
<td>2.8–6.3</td>
</tr>
<tr>
<td>Width (m)</td>
<td>1.67–1.83</td>
<td>Pump pressure (Mpa)</td>
<td>31.5</td>
</tr>
<tr>
<td>Setting load (kN)</td>
<td>1648–4068</td>
<td>Oscillation angle of tilt beam (°)</td>
<td>35–65</td>
</tr>
<tr>
<td>Working resistance (kN)</td>
<td>10627–11207</td>
<td>Top beam length (m)</td>
<td>3.12</td>
</tr>
<tr>
<td>Support intensity (MPa)</td>
<td>1.25–1.32</td>
<td>Support weight (t)</td>
<td>42.6</td>
</tr>
<tr>
<td>Pressure of base (Mpa)</td>
<td>2.04–2.45</td>
<td>Roof-control distance (m)</td>
<td>6.5</td>
</tr>
</tbody>
</table>

Table II
The standard value and variation of each parameter

<table>
<thead>
<tr>
<th>Parameter</th>
<th>α (°)</th>
<th>L (m)</th>
<th>f1</th>
<th>f2</th>
<th>B (m)</th>
<th>H (m)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Average</td>
<td>12</td>
<td>1.2</td>
<td>0.2</td>
<td>1.75</td>
<td>6</td>
<td></td>
</tr>
<tr>
<td>Range</td>
<td>5–25</td>
<td>0.5–1.6</td>
<td>0.1–0.3</td>
<td>1.67–1.83</td>
<td>4.0–6.5</td>
<td></td>
</tr>
<tr>
<td>Average</td>
<td>7000</td>
<td>0.4</td>
<td>2</td>
<td>50</td>
<td>15</td>
<td></td>
</tr>
<tr>
<td>Range</td>
<td>0–8800</td>
<td>0.22–0.82</td>
<td>1.7–2.6</td>
<td>35–65</td>
<td>12–18.3</td>
<td></td>
</tr>
</tbody>
</table>

Table III
Sensitive parameters that affect stability capability of HSG

<table>
<thead>
<tr>
<th>Parameter</th>
<th>α</th>
<th>f1</th>
<th>f2</th>
<th>P</th>
<th>Sensitivity</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sensitivity</td>
<td>1.4295</td>
<td>0.4142</td>
<td>0.6151</td>
<td>0.4142</td>
<td></td>
</tr>
</tbody>
</table>

Table IV
Sensitive parameters that affect stability capability of HST

<table>
<thead>
<tr>
<th>Parameter</th>
<th>α</th>
<th>f1</th>
<th>h</th>
<th>P</th>
<th>C</th>
<th>B</th>
<th>Sensitivity</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sensitivity</td>
<td>1.43</td>
<td>0.5612</td>
<td>0.0896</td>
<td>0.1175</td>
<td>0.0343</td>
<td>0.0076</td>
<td></td>
</tr>
</tbody>
</table>

Table V
Sensitive parameters that affect stability capability of HST

<table>
<thead>
<tr>
<th>Parameter</th>
<th>α</th>
<th>f1</th>
<th>f2</th>
<th>f3</th>
<th>H</th>
<th>Sensitivity</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sensitivity</td>
<td>1.4295</td>
<td>0.2978</td>
<td>0.7373</td>
<td>1</td>
<td>0.04</td>
<td>0.076</td>
</tr>
</tbody>
</table>

The parameters can be classified into three categories – sensitive parameters (S≥0.5), less-sensitive parameters (0.1≤S<0.5), and non-sensitive parameters (S<0.1) (Yuan, 2011; Zhang and Zhu, 1993).

In the anti-gliding condition, α and f2 are sensitive parameters, and f1 and P are less-sensitive parameters. In the anti-gliding condition, α and f1 are sensitive parameters, with P being less sensitive and h, C, and B being non-sensitive parameters. In the anti-tail tilting condition, α, f2, f3, P, and θ are sensitive parameters, f1, H, L, and Ld are less-sensitive parameters, and B is the non-sensitive parameter. The relationships between the hydraulic support stability coefficient and the sensitivity are shown in Figures 4, 5, and 6, derived using the MATLAB software package.

Figures 4, 5, and 6 indicate that:

indicates that U is very sensitive to βk, and βk can be termed a hypersensitive parameter. Otherwise, βk is a less-sensitive parameter.

For purposes of comparison with each property-different and unit-different parameter, a dimensionless sensitive factor is defined as follows:

\[ S(β_k) = \max \left( \frac{A_{β_k - \max} - A^*}{A^* - A_{β_k - \min}} \right) \]  \[ \text{[22]} \]

where \( S(β_k) \) is the sensitivity of \( β_k \); \( A^* \) is the corresponding characteristic value of criterion parameter set; and \( A_{β_k - \max} \) and \( A_{β_k - \min} \) are the maximum and minimum characteristic values varying in the range of \( β_k \), respectively.

Multi-parameter SAM of HSI in FMMLMH

The no.7219 working face in Xutuan Mine is used as an example. The coal seam thickness ranges from 4.0 to 6.5 m, with an average of 6.0 m, and the dip of the seam varies from 5° to 25°, with an average of 12°. The hydraulic support system used is ZY11000/28/63, and the main technical parameters are listed in Table I.

Eleven parameters are selected to analyse their influence on HSI, i.e. \( f_1, f_2, f_3, P, h, B, H, L, L_d, \) and \( θ \). Using the geological conditions, the ground pressure observations at the working face, and the parameters in Table I, the average value and range of variation for each parameter are listed in Table II. The the average value and variation range of the 11 parameters are derived as follows. The parameters of \( α \) and \( h \) are obtained from the geological conditions of the working face; \( P \) and \( H \) are derived from field measurement of strata behavior; \( B, L, L_d, \) and \( θ \) are acquired from the technical parameters of the ZY11000/28/63 hydraulic support; and \( f_1, f_2, \) and \( f_3 \) are obtained from Gong and Jin (2001), Yuan et al. (2008), and Yuan (2011).

The sensitive parameters, derived by using SAM, that affect the support stability in the no.7219 working face are listed in Tables III, IV, and V.
Hydraulic support instability mechanism

Figure 4 – Relationship between sensitive parameters (α and $f_2$) and anti-HSG stability coefficient ($K_h$)

Figure 5 – Relationship between sensitive parameters (α and $f_1$) and anti-HST stability coefficient ($K_d$)

Figure 6 – Relationship between sensitive parameters (α, $f_2$, $f_3$, $P$ and $\theta$) and anti-HSTT stability coefficient ($K_n$)
Hydraulic support instability mechanism

- The anti-HSTT stability coefficient $K_0$ is relatively high, indicating that HSG and HST are the main HSI forms in the no.7219 working face.
- The parameters of $\alpha$ and $f_2$ have a greater impact on the anti-gliding stability coefficient $K_0$ compared with $f_1$ and $P$. To avoid HSG, it is essential to increase the value of $f_2$ or to decrease the value of $f_1$, for example, by making the layout of the working face with apparent dip and step pattern floor. Increasing the values of $f_1$ or $P$ is also an effective way to prevent HSG, for example, by moving the hydraulic support under pressure.
- The anti-tilting stability coefficient $K_T$ is fairly sensitive to $f_1$, therefore emplacing the hydraulic support temporarily after moving the support is an effective way to prevent HSG.

Conclusions

Hydraulic support instability (HSI) is likely to occur on steeply dipping coal seam working faces where fully-mechanized mining with a large mining height (FMMLMH) is applied. In order to control HSI, the mechanism of HSI in FMMLMH was modelled and interpreted, and the critical instability angles for the three HSI forms, i.e. hydraulic support gliding (HSG), hydraulic support tilting (HST), and hydraulic support tail twisting (HSTT) were obtained.

HSI in FMMLMH is a complex system issue influenced by 11 factors. Sensitivity analysis is an effective way to analyse the sensitivity of these factors and improve the effectiveness of hydraulic support stability control.

The multi-parameter sensitivity analysis of HSI in the no.7219 working face indicated that HSG and HST are the two main instability forms for HSI, as the anti-HSTT stability coefficient in this working face is relatively high. HSG is sensitive to the dip angle of the working face and the friction coefficient between floor and hydraulic support, while the dip angle of the working face and the friction coefficient between roof and hydraulic support are the main controlling parameters for HST. Through the above analysis, the oblique layout of the working face, step pattern of the floor, timely advance of support under pressure, and raising the setting load are the main technical measures to improve the support stability in the no.7219 working face, which contribute to the safety and efficiency of mining operations.

Acknowledgments

Financial support for this work was provided by the Priority Academic Program Development of Jiangsu Higher Education Institutions, and the Fundamental Research Funds for the Central Universities (No. 2014QNB32).

References


Liu, J.F. 2006. Study on adaptability of shield support in large cutting height working face. *Coal Science Research Institute, Beijing*.


Yuan, Y. 2011. Stability control mechanism of support-surrounding rocks at fully mechanized mining face with great cutting height. *China University of Mining and Technology, Xuzhou*.


OBJECTIVES
The conference will focus on improving health, safety and the environmental impact in the mining and metallurgy industry and highlight actions to be taken. It will act as a platform for learning and allow people to share ideas on safety, health and the environment.

This conference aims to bring together management, DMR, Chamber of Mines, Unions and health and safety practitioners at all levels from the industry to share best practice and successful strategies for zero harm and a value-based approach to health and safety. It will address the main challenges in the mining industry such as logistics, energy and safety of employees, contractors and the communities.

SPONSORSHIP
Sponsorship opportunities are available. Companies wishing to sponsor or exhibit should contact the Conference Coordinator.

WHO SHOULD ATTEND
The conference should be of value to:
- Safety practitioners
- Mine management
- Mine health and safety officials
- Engineering managers
- Underground production supervisors
- Surface production supervisors
- Environmental scientists
- Minimizing of waste
- Operations manager
- Processing manager
- Contractors (mining)
- Including mining consultants, suppliers and manufacturers
- Education and training
- Energy solving projects
- Water solving projects
- Unions
- Academics and students
- DMR
- Acid mine drainage.

For further information contact:
Head of Conferencing
Raymond van der Berg, SAIMM,
P O Box 61127, Marshalltown 2107
Tel: +27 11 834-1273/7
Fax: +27 11 833-8156 or +27 11 838-5923
E-mail: raymond@saimm.co.za
Website: http://www.saimm.co.za
Introduction

In recent years, stoping methods have been magnified as an extraction strategy in underground hard rock mining. According to a report from AusTrade (2013), in 2013 70% of underground metal mines in Australia utilized open stoping, sublevel stoping, various narrow stoping methods, and other types of stoping and caving methods to extract ore. In addition, 51% of underground metal production in Canada relies on open stoping methods (Pakalnis et al., 1996). A disadvantage of popular stoping methods is that many mines are severely affected by dilution problems. Pakalnis (1986) surveyed 15 open stope Canadian mines and concluded that 47% of the operations suffered from more than 20% dilution. Likewise, Henning and Mitri (2007) reported that approximately 40% of open stoping operations in Canada suffered from 10% to 20% dilution.

Dilution can be defined as ‘the contamination of ore with lower grade material’, and it can be generally classified into two categories: planned and unplanned. Planned dilution, also referred to as primary or internal dilution, is contamination by low-grade material within the ore block; whereas unplanned dilution, also known as secondary or external dilution, is contamination by lower grade material exterior to the ore block. Both of these dilute the ore stream value. Ore loss can similarly be classified as planned and unplanned. Planned ore loss represents the ore-grade material that has been excluded from the mining block at the stope design stage, whereas unplanned ore loss is the part of the mining block that remains in the stopes after mining.

This study includes unplanned dilution and ore loss, which can be attributed to over- and underbreak in underground stoping production. These phenomena can be divided into dynamic and quasi-static types; the quasi-static type occurs after blasting, while the dynamic type occurs immediately (Mandal and Singh, 2009). The dynamic over- and underbreak types are the main interest of this study, and a new terminology, ‘uneven break’ (UB), is used to identify it. To extend the definition of dilution, UB can be defined as the tons of mined unplanned dilution (positive) or ore loss (negative) per ton of ore mined, expressed as a percentage.

\[
\text{UB rate} = \frac{\text{tons of unplanned dilution or ore loss/tons ore mined}}{} \times 100 \quad [1]
\]

UB affects not only the safety of the workforce and machinery, but is also severely detrimental to the viability of the operation throughout all of the mining stages. It directly downgrades the ore and causes unnecessary mucking, haulage, crushing, hoisting, and milling activities, thus decreasing productivity. Despite these effects, current UB management

Unplanned dilution and ore loss prediction in longhole stoping mines via multiple regression and artificial neural network analyses

by H. Jang*, E. Topal*, and Y. Kawamura*

Synopsis

Unplanned dilution and ore loss directly influence not only the productivity of underground stopes, but also the profitability of the entire mining process. Stope dilution is a result of complex interactions between a number of factors, and cannot be predicted prior to mining. In this study, unplanned dilution and ore loss prediction models were established using multiple linear and nonlinear regression analysis (MLRA and MNRA), as well as an artificial neural network (ANN) method based on 1067 data-sets with ten causative factors from three underground longhole stoping mines in Western Australia. Models were established for individual mines, as well as a general model that includes all of the mine data-sets. The correlation coefficient (R) was used to evaluate the methods, and the values for MLRA, MNRA, and ANN compared with the general model were 0.419, 0.438, and 0.719, respectively. Considering that the current unplanned dilution and ore loss prediction for the mines investigated yielded an R of 0.088, the ANN model results are noteworthy. The proposed ANN model can be used directly as a practical tool to predict unplanned dilution and ore loss in mines, which will not only enhance productivity, but will also be beneficial for stope planning and design.

Keywords

stoping, unplanned dilution, ore loss, artificial neural network.

* Department of Mining Engineering and Metallurgical Engineering, Western Australian School of Mines, Curtin University, Australia.

The Journal of The Southern African Institute of Mining and Metallurgy

VOLUME 115

MAY 2015

449
Unplanned dilution and ore loss prediction in longhole stoping mines

relies on previous production results from similar stopes and veteran engineers’ intuitions. UB has been considered an unavoidable and unpredictable phenomenon in practice due to the extremely complex mechanism of interaction between the many causative factors.

In this study, new UB prediction models are established through multiple linear and nonlinear regression analysis (MLRA and MNRA) as well as an artificial neural network (ANN) method. The data was collected from three underground longhole stoping mines in Western Australia. The UB prediction models were established for individual mine sites. Moreover, entire data-sets were used to propose a general model to predict UB. The proposed models are compared with actual stope dilution and the current UB predictions for mines.

Overview of unplanned dilution and ore loss in stoping

Unplanned dilution and ore loss directly affect the profitability of mining and are the most critical factors affecting the economics of underground stoping. The importance of unplanned dilution and ore loss control has been emphasized by many researchers. Tatman (2001) reported that reducing unplanned dilution is the most effective way to increase mine profits, and Henning and Mitri (2008) stressed the significant influence of unplanned dilution on the profitability of mining operations. More specifically, in 2008, Stewart and Trueman (2008) reported that unplanned dilution costs A$25 per ton, compared with A$7 per ton for mucking and haulage, and A$18 per ton for milling in typical narrow-vein longhole stoping operations. Suglo and Opoku (2012) conducted a study on Kazanski Mine and calculated the financial loss from unplanned dilution during 1997 to 2006 at US$45.98 million. In 2002, US$11.30 million was spent to control unplanned dilution at the Konkola Mine in Zambia (Mubita, 2005).

Previous studies on unplanned dilution and ore loss control

Unplanned dilution and ore loss have been investigated by many researchers, but a practical prediction model that considers a broad range of causative parameters has not been introduced until now. Most of the previous studies have attempted to discover the relationship between unplanned dilution and a few particular causative factors.

Germain and Hadjigeorgiou (1997) used simple linear regression to analyse stope overbreak at the Louvicourt Mine in Canada. The stope performances were recorded by a cavity monitoring system (CMS), and the actual stope geometries and blasting patterns were recorded. The authors concluded that the relationship between stope performance and other dependent parameters is very complex, and the correlation coefficient (\( R \)) values for the powder factor and Q-value were only -0.083 and 0.282, respectively. Despite this data, the stope volume showed a moderate positive correlation with the ratio between stope volume and its real surface area (RVS). Wang et al. (2002) found that dilution was greater for a parallel drilling pattern than for a fanned pattern, while Clark and Pakalnis (1997) reported that dilution tended to increase when blast-holes fanned out. Stewart (2005) demonstrated the difficulties of predicting unplanned dilution by comparing the conflicting results; opposing observations on the unplanned dilution problem are common and evident when an aspect of the unplanned dilution problem is restricted to a few causative parameters.

Henning and Mitri (2007) used a three-dimensional elastic-plastic numerical analysis program (Map3D) to examine the influence of depth, in-situ stress, and stope geometry on the stope wall overbreak. The authors considered two criteria: the area of zero tensile strength (\( \sigma_3 = 0 \)) and the tensile strength of the rock mass (\( \sigma_3 = \sigma_t \)). The contour of the relaxation zone (\( \sigma_3 = 0 \)) remained nearly constant, while the potential overbreak associated with the rock mass tensile strength increased with depth for a given stope geometry or hangingwall dip. Subsequently, the influence of the mining sequencing on blast-hole stoping dilution was studied (Henning and Mitri, 2008) in 172 sequentially mined longhole stopes. The authors concluded that the overbreak significantly increased in stopes that had one or more backfilled walls.

Recently, the stability graph method (Mathews et al., 1981; Potvin, 1988) has been commonly used to design and manage stope stability. The stability graph method is a useful tool for constructing a site-specific database, and some authors have indicated that it may facilitate stope dilution prediction (Diederichs and Kaiser, 1996; Pakalnis et al., 1996). Despite of the popularity of the stability graph method, some limitations have been pointed out by several researchers. Martin et al. (1999) stated that the far field stress with respect to the stope orientation has not been considered. In addition, Potvin and Hadjigeorgiou (2001) noted that the method is not appropriate for controlling rockburst conditions. Furthermore, the method does not consider any blasting factors, induced stress by stope developing sequences, and the exposure time of the stope wall. Essentially, the UB could not be predicted in practice using the stability graph method itself. For instance, the stability graph method was also used at the three mines in the current investigation as a guideline for stope design and a tool to predict unplanned dilution. The predicted performances are shown in Table I.

As shown in Table I, the UB predictions were extremely...
unsatisfactory and were limited to only unplanned dilution, but not ore loss. In addition, comparisons between the actual and current predicted unplanned dilution as well as the current UB predictions for the general model are shown in Figure 1.

Despite significant research effort, UB is still considered an unpredictable phenomenon. This study provides an optimistic perspective on predicting the potential UB using the advanced artificial neural network method.

Factors that influence unplanned dilution and ore loss
UB can be defined as a dynamic-type over- and underbreak that corresponds to unplanned dilution and ore loss. Numerous interacting factors affect UB. Thus, the mechanism underlying UB cannot be properly analysed based only on a single causative factor or a group of factors, but it is imperative to consider the entire range of factors that may contribute.

Several researchers (Clark, 1998; Henning and Mitri, 2007; Mathews et al., 1981; Mubita, 2005; Potvin, 1988; Stewart, 2005; Tatman, 2001; Villaescusa, 1998; Yihong and Weijin, 1986) have indicated that the factors that are likely to cause unplanned dilution and ore loss can be divided into three core groups with one subsidiary group (i.e. blasting, geological, stope design, and human error and others). Certain representative recommendations were classified into four groups and are summarized in Table II.

Data collection
Data collection is a herculean task but vital for this study, and the prediction capability of the proposed model fully relies on the data quality. To avoid potential bias and establish appropriate UB prediction models, the extensive range of historical stope reconciliation data and geological data was scrutinized. Initially, 1354 data-sets with 45 parameters in three core causative categories were collected via a thorough review of over 30 000 historical documents from three underground longhole and open stoping mines in Western Australia. Ultimately, ten parameters were used as the representative causative factors for UB. Figure 2 is an overview of one investigated mine with an example of stope reconciliation data using a cavity monitoring system (CMS).

As shown in Figure 2, the planned stope model was compared with the actual stope model, which was obtained using the CMS. The unplanned dilution volume and ore loss percentage were calculated not only for the hangingwall but also for the footwall. The geology, stope design, and blasting data were collected in succession through examining corresponding documents.

For a coherent analysis, 287 abnormal data-sets were removed through examining univariate, bivariate, and multivariate outliers because they could influence the analysis in various ways and decrease the reliability of the proposed model.

Multiple regression analysis
Initial, all independent variables were forced into the MLRA model, which is referred to as the MLRA-enter model. Next, the insignificant variables were progressively removed to such as blast-hole deviation and drilling error were impossible to obtain. Thus, the average blast-hole length (Blen) data was collected to indirectly compute the blast-hole deviation, because drilling accuracy for longhole drilling is generally expressed as a percentage of the blast-hole depth (Stiehr and Dean, 2011).
Unplanned dilution and ore loss prediction in longhole stoping mines

Table II
Summary from representative studies on causative factors for UB

<table>
<thead>
<tr>
<th>Reference</th>
<th>Geological</th>
<th>Blasting</th>
<th>Stope design</th>
<th>Human error and others</th>
</tr>
</thead>
<tbody>
<tr>
<td>Potvin (1988)</td>
<td>Block size, stress, joint orientation, and gravity support</td>
<td>Blasting practice</td>
<td>Stope geometry</td>
<td>Backfill and adjacent stope timing</td>
</tr>
<tr>
<td>Villaescusa (1998)</td>
<td>Poor geological control Inappropriate support schemes</td>
<td>Poor initial blast geometry Incorrect blast patterns Sequences of explosive types</td>
<td>Poor stope design Lack of proper stope sequencing</td>
<td>Deviation of blast-holes Lack of supervision &amp; communication Rushed stope planning and lack of stope performance review</td>
</tr>
<tr>
<td>Clark (1998)</td>
<td>Rock quality and major structures stress</td>
<td>Blast-hole geometry Up- and down-holes Breakthroughs Parallel and fanned holes Explosive types Blast sequences</td>
<td>Undercutting Stopping sequence, supports, and geometry Hydraulic radius Slot raise location</td>
<td>Realistic collar location Blast-hole deviation Communication between engineers</td>
</tr>
<tr>
<td>Tatman (2001)</td>
<td>Less-than-ideal wall condition</td>
<td>High powder factor</td>
<td>Improperly aligned drill-holes</td>
<td>Equipment limitations</td>
</tr>
<tr>
<td>Mubita (2005)</td>
<td>Inadequate ground condition</td>
<td>Poor blasting results</td>
<td>Stope boundary inconsistencies Inappropriate mining methods</td>
<td>Poor mining discipline</td>
</tr>
<tr>
<td>Stewart (2005)</td>
<td>Stress damage pillars</td>
<td>Blasting damage</td>
<td>Site-specific effects Undercutting Extraction sequence</td>
<td>Backfill abutment Damage to cemented fill</td>
</tr>
<tr>
<td>Factors employed in this study</td>
<td>Adjusted Q-rate Average horizontal to vertical stress ratio</td>
<td>Length of blast-hole Powder factor Angle difference between hole and wall Diameter of blast-hole Space and burden ratio</td>
<td>Planned tons of stope Aspect ratio Stope breakthrough to a nearby drift/stope or not</td>
<td>Indirectly implied blast-hole deviation through the average blast-hole length</td>
</tr>
</tbody>
</table>

Table III
Description and summary of the ten UB causative factors

<table>
<thead>
<tr>
<th>Category</th>
<th>Abbr.</th>
<th>Unit</th>
<th>Range</th>
<th>Note</th>
</tr>
</thead>
<tbody>
<tr>
<td>Input (independent variables)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Blasting</td>
<td>Blen</td>
<td>m</td>
<td>0.70 ~ 25.80</td>
<td>Average length of blast-hole</td>
</tr>
<tr>
<td></td>
<td>Pf</td>
<td>Kg/t</td>
<td>0.15 ~ 3.00</td>
<td>Powder factor</td>
</tr>
<tr>
<td></td>
<td>AHW</td>
<td>°</td>
<td>0.00 ~ 170.20</td>
<td>Angle difference between hole and wall</td>
</tr>
<tr>
<td></td>
<td>Bdia</td>
<td>mm</td>
<td>76 ~ 89</td>
<td>Diameter of blast-hole</td>
</tr>
<tr>
<td></td>
<td>SbR</td>
<td>(S/B)</td>
<td>0.57 ~ 1.50</td>
<td>Space(S) and burden(B) ratio</td>
</tr>
<tr>
<td>Geology</td>
<td>AQ</td>
<td>(H/V)</td>
<td>6.30 ~ 93.30</td>
<td>Adjusted Q rate</td>
</tr>
<tr>
<td></td>
<td>K</td>
<td></td>
<td>1.0 ~ 14.38</td>
<td>Average horizontal (H) to vertical (V) stress ratio</td>
</tr>
<tr>
<td>Stope design</td>
<td>Pt</td>
<td>T</td>
<td>130 ~ 61,450</td>
<td>Tons of stope planned</td>
</tr>
<tr>
<td></td>
<td>AsR</td>
<td>(W/H)</td>
<td>0.07 ~ 4.17</td>
<td>Aspect ratio (ratio between width (W) and height (H) of stope)</td>
</tr>
<tr>
<td></td>
<td>BTBL</td>
<td>-</td>
<td>Breakthrough (0) ~ Blind (1)</td>
<td>Stope breakthrough to a nearby drift/stope, or not</td>
</tr>
<tr>
<td>Output (dependent variable)</td>
<td>UB</td>
<td>%</td>
<td>-85.40 ~ 92.00</td>
<td>Percentage of uneven stope break (over- and under-break)</td>
</tr>
</tbody>
</table>

obtain the optimised MLRA-stepwise model based on the statistical significance levels for $F$ and $t$ values. The MLRA-enter and stepwise model results are shown in Table IV. As can be seen from Table IV, for the Mine A data-set, the adjusted coefficients of the determinant ($R^2_{adj}$) for the MLRA-enter and stepwise models were 0.280 and 0.293, respectively. The $K$, Blen, Hdia, BTBL, and SbR were removed from the MLRA-stepwise model due to their low $t$-value significance levels. The Mine B data-set MLRA models yielded the highest $R^2_{adj}$ values among the MLRA models; the MLRA-enter and stepwise models yielded 0.322 and 0.330, respectively. Hdia was not considered in the models because the Mine B data-set had only one value for this variable. The $t$-values for BTBL, ShR, Pt, Pf, and AsR were inadequate; they were therefore removed from the MLRA-stepwise model. The MLRA-enter and stepwise models for Mine C had the lowest adjusted coefficients of the determinant ($R^2_{adj}$), 0.166 and 0.163, respectively. The $F$ and $t$ values for $K$, Hdia, ShR,
Unplanned dilution and ore loss prediction in longhole stoping mines

When multiple regression analysis is applied, heteroskedasticity and multicollinearity problems must be considered because they may yield an erroneous conclusion. In this study, no suspicious results were found from the MLRA-stepwise and MNRA models through checking the residual plots, variance inflation factor (VIF), and the Durbin-Watson value (Durbin and Watson, 1950).

Multiple nonlinear regression analysis

Dilution and ore loss are the most complex phenomena in underground mining production, and they are affected by various factors as described previously. The complex phenomena cannot be fully interpreted using a linear model. Thus, MNRA was performed to obtain more significant relationships than from the MLRA. In this study, the twin-logarithmic model was used, and the following nonlinear relation was assumed:

\[
Y = \beta_0 (X_1^{\beta_1})(X_2^{\beta_2})...(X_n^{\beta_n})
\]

[2]

where \(Y\) denotes the predicted value corresponding to the dependent variables \(X_1, X_2, ..., X_n\), and \(\beta_0\) to \(\beta_n\) are the parameters for the nonlinear relationship. Equation [2] can be transformed into a linear domain through log transformation as shown in Equation [3]; thus, the \(\beta\) values can be determined based on a multiple linear regression of \(\log(Y)\) on \(\log(X_1), \log(X_2), ..., \log(X_n)\) (Cankaya, 2009).

\[
\log(Y) = \log(\beta_0) + (\beta_1 \log(X_1) + \beta_2 \log(X_2) + \ldots + \beta_n \log(X_n))
\]

[3]

The dependent variable (UB) has negative values that express the ore loss rate; and two independent variables (BTBL and AHW) contain zero values. The negative and zero values cannot be applied to the logarithmic function. Hence, the data-sets must be transformed into positive, real values. For data-sets containing zero and negative values, the following nonlinear relation was assumed:

\[
Y = \beta_0 - \beta_1 X_1^{\beta_2} - \beta_3 X_2^{\beta_4} - \ldots - \beta_n X_n^{\beta_n}
\]

[4]

\(Y\) denotes the predicted value corresponding to the dependent variables \(X_1, X_2, ..., X_n\), and \(\beta_0\) to \(\beta_n\) are the parameters for the nonlinear relationship. Equation [4] can be transformed into a linear domain through log transformation as shown in Equation [5]; thus, the \(\beta\) values can be determined based on a multiple linear regression of \(\log(Y)\) on \(\log(X_1), \log(X_2), ..., \log(X_n)\) (Cankaya, 2009).

\[
\log(Y) = \log(\beta_0) + (\beta_1 \log(X_1) + \beta_2 \log(X_2) + \ldots + \beta_n \log(X_n))
\]

[5]

The dependent variable (UB) has negative values that express the ore loss rate; and two independent variables (BTBL and AHW) contain zero values. The negative and zero values cannot be applied to the logarithmic function. Hence, the data-sets must be transformed into positive, real values. For
an unbiased transformation, unity was added after the data-sets were normalized between zero and one. Thus, the data-sets yielded values between one and two. MNRA was accomplished using the Levenberg-Marquardt iterative estimation algorithm (Marquardt, 1963). Subsequently, optimal models for Mine A, Mine B, Mine C, and the general model were obtained after eight, twelve, six, and six iterations, when the residual sum of squares reached 1.0E-008. The MNRA model results are shown in Table V.

The adjusted coefficients of the determinant ($R_{adj}^2$) for Mine A, Mine B, Mine C, and the general model were 0.317, 0.368, 0.181, and 0.192, which are slightly higher than from the MLRA-stepwise models. In fact, the MNRA models were also insufficient for clarifying the relationship between the UB and given independent variables.

## Artificial neural network

An artificial neural network (ANN) can be defined as a parallel computational inference model whose functionality is simply mimicked by a biological neuron. The fundamental structure of an ANN comprises input, hidden, and output layers and numbers of a simple mathematical element, the artificial neurons, which are in each layer. The neurons are fully interconnected to each layer, and the connection intensity is expressed by the weight. The optimum weight of all connections can be obtained through continuous forward and backward processes with a certain learning algorithm during the training stage. Next, a new set of inputs can yield a prediction only through the forward process with the optimized weight from the previous training. Indeed, the ANN is optimized by simply discovering the optimum weights of the model connections. The structure of the multilayer feed-forward ANN used in this study can be seen in Figure 3.

In the proposed ANN model, the conjugate gradient algorithm (CGA) (Hestenes and Stiefel, 1952) was applied as an learning algorithm of the ANN model and the weights can be updated as follows:

$$w_{p+1} = w_p - g \cdot \nabla E(w_p) + \beta_{p+1} \cdot g_p$$

where $w_{p+1}$ indicates the updated weight for $p+1$ step, $g$ is the error gradient ($g = \frac{\partial E(x, w)}{\partial w}$), and $\beta_{p+1}$ is the conjugate gradient algorithm constant. In the CGA, the search direction is determined with a conjugate direction that generally yields more rapid convergence than with the steepest descent (Møller, 1993). Various types of combination coefficients ($\beta$) were introduced to determine the appropriate conjugate direction. A well-known algorithm was introduced by Fletcher and Reeves (1964), and the $\beta$ for $p+1$ step can be calculated as follows:

$$\beta_{p+1} = \left( g^T_p \cdot g_{p+1} \right) / \left( g^T_p \cdot g_p \right)$$

### Table V

<table>
<thead>
<tr>
<th>Data-sets</th>
<th>Model</th>
<th>Equation</th>
<th>$R$</th>
<th>$R_{adj}^2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mine A</td>
<td>MNRA</td>
<td>$UB = 1.407(PT^{0.09}(AHW-0.40)(AQ-0.50)(PT-0.35)(AsR-0.42)$</td>
<td>0.56</td>
<td>0.317</td>
</tr>
<tr>
<td></td>
<td>Selected2</td>
<td>$K, Blen, Hdia, BTBL, and SbR$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Mine B1</td>
<td>MLRA</td>
<td>$UB = 1.669(Blen-16)(AHW-162)(AQ-85.9)(K-1.259)$</td>
<td>0.60</td>
<td>0.368</td>
</tr>
<tr>
<td></td>
<td>Selected</td>
<td>$BTBL, SbR, Pt, and AsR$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Mine C</td>
<td>MLRA</td>
<td>$UB = 1.455(BTBL-0.39)(Blen-129)(AHW-102)(AQ-12)(AsR-167)$</td>
<td>0.425</td>
<td>0.181</td>
</tr>
<tr>
<td></td>
<td>Selected</td>
<td>$K, Hdia, SbR, and Pt$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>General</td>
<td>MLRA</td>
<td>$UB = 1.473(BTBL-0.37)(Blen-110)(PT-107)(AHW-144)(AQ-112)(AsR-0.79)$</td>
<td>0.428</td>
<td>0.192</td>
</tr>
<tr>
<td></td>
<td>Selected</td>
<td>$K, Hdia, SbR, and Pt$</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

1. Hdia was removed from the MLRA and MNRA because the Mine B data-set had only one value for this variable.
2. Selected: independent variables were selected from the –MLRA-stepwise model.

Figure 3 – Architecture of the multilayer feed-forward ANN model for the UB prediction system
Unplanned dilution and ore loss prediction in longhole stoping mines

Results and discussion

MLRA, MNRA, and ANN were used to develop the optimum UB prediction model based on 1067 data-sets with ten UB causative factors from three longhole stoping underground mines in Western Australia. The UB prediction model was established not only for each mine, but also for all of the mine data-sets. Ultimately, the MLRA, MNRA, and ANN prediction performances were compared with the current prediction mine results (Figure 5).

As can be seen from Figure 5, the MLRA and MNRA models yielded poor and moderate UB prediction performances. Their correlation coefficients \( R \) were between 0.412 and 0.607. In contrast to multiple regression analyses, the ANN models yielded fair and excellent UB prediction performances. The correlation coefficients \( R \) for Mine A, Mine B, and Mine C were 0.944, 0.801, and 0.704, respectively. The general model for ANN was trained with 747 data-sets, and 160 untrained data-sets were used to validate the system during the training process to prevent over-fitting. Ultimately, the optimized ANN model was established with the RMSE of 1.90E-2 and tested with 160 untrained data-sets. The correlation coefficient \( R \) for the test was 0.719.

Table VI

<table>
<thead>
<tr>
<th>Model</th>
<th>Number of data-sets</th>
<th>Structure of ANN</th>
<th>RMSE(^4)</th>
<th>( R^5 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mine A</td>
<td>88</td>
<td>10 – 7 – 1</td>
<td>1.04E-2</td>
<td>0.92</td>
</tr>
<tr>
<td>Mine B</td>
<td>161</td>
<td>10 – 16 – 1</td>
<td>2.15E-2</td>
<td>0.86</td>
</tr>
<tr>
<td>Mine C</td>
<td>496</td>
<td>10 – 16 – 1</td>
<td>2.36E-2</td>
<td>0.74</td>
</tr>
<tr>
<td>General model</td>
<td>747</td>
<td>10 – 40 – 1</td>
<td>1.90E-2</td>
<td>0.66</td>
</tr>
</tbody>
</table>

\(^4\)RMSE: root mean square error; \(^5\)R: correlation coefficient

Figure 4 – Test performance of UB prediction ANN models for Mine A, Mine B, Mine C, and the general model

In all models, the training and validation RMSE decreased dramatically within 30 iterations, and it gradually reduced through 100 iterations. The optimum number of hidden neurons for the ANN model for Mine A, Mine B, Mine C, and the general model were 7, 16, 16, and 40 respectively. The RMSE for the training stages was less than 2.36E-2, and strong positive correlations \( R > 0.7 \) were observed. Figure 4 illustrates test performance graphs of each model.

Considering that UB has been neglected as an unpredictable phenomenon, these results are noteworthy. The result will be thoroughly scrutinized for comparison with the current UB prediction results for mines in the following section.
Unplanned dilution and ore loss prediction in longhole stoping mines

The proposed ANN engine can be easily applied to underground stoping mines because the input parameters of the proposed ANN are generally collected for each underground stope. Engineers can examine potential unplanned dilution and ore loss prior to the actual stope development by inputting these parameters to the proposed ANN.

Conclusions

New unplanned dilution and ore loss prediction models were established using multiple linear regression analysis (MLRA), multiple nonlinear regression analysis (MNRA), and an artificial neural network (ANN) method for 1067 historical stope data-sets collected from three underground longhole stoping mines in Western Australia. Models were established not only for each mine but also for the data-sets as a whole to propose a general model for predicting UB. Correlation coefficients (R) were used to evaluate the MLRA, MNRA, and ANN performance; their values for the general model were 0.419, 0.438, and 0.719, respectively. Considering the current UB prediction in investigated mines yielded an R of 0.088, the ANN model results are significant.

Although the exact causes of unplanned dilution and ore loss are extremely complex, the general trends underlying the UB mechanism were somewhat elucidated using the ANN model. The established ANN models were calibrated using untrained data-sets during the test stage. Thus, they can be directly used as a tool for practical prediction for any underground longhole stoping operation. As such, this paper will create significant benefit for underground stope planning and design.

References


Numerical simulation of multiphase flow in a Vanyukov furnace

by H.L. Zhang*, C.Q. Zhou†, W.U Bing†, and Y.M. Chen*

Synopsis
Multiphase flow in the widely used Vanyukov furnace was numerically studied. An unsteady three-dimensional and three-phase flow model was firstly built using the computational fluid dynamics (CFD) software ANSYS FLUENT®, and then solved with the volume of fluid (VOF) and \( k - \varepsilon \) model. The results showed that the proposed model could be used to predict the multiphase movement, the slag/air fluctuation, the vortex formation, and effects of structural and operational parameters. By fast Fourier transform (FFT), the dominant frequency of density with time signal was calculated as 0.29 Hz. The analysis of different injection flow rates of enriched air indicated that this variable has a major effect on the mean slag velocity. The peak mean velocity increased from 2.17 to 4.99 m/s while the flow rate of enriched air varied from 70 to 160 m/s. The proposed model provides a method to optimize the furnace structure and operating conditions for the best furnace performance and lowest energy consumption.

Keywords
Vanyukov furnace, multiphase flow, numerical simulation, fast Fourier transform, structure optimization, operation condition optimization.

Introduction
The main technologies adopted in the copper and lead reduction industries include the Vanyukov, QSL, SKS, Kivcet, Ausmelt, and ISA furnaces (Hongjiu, 2001; Kojo, Jokilaakso, and Hanniala, 2000). From a fundamental theoretical viewpoint, all of these technologies can be classified as reduction bath smelting furnaces, which are the major research focus in nonferrous metallurgy. However, some of the important physical phenomena and chemical processes inside the furnace remain unknown because of the harsh reaction environments. Fortunately, numerical simulation methods, particularly computational fluid dynamics (CFD), provide an efficient way to study their internal processes.

With the development of computer software, many good CFD platforms have been released, such as Fluent and CFX. CFD has become an indispensable tool for the design and optimization of complex chemical reactors. Typical applications included the blast furnace (BF) and aluminum reduction cell. In the copper industry, some papers have been published on numerical studies of the flow pattern. The representative work in this area was carried out by Valencia and co-workers at the Institute for Innovation in Mining and Metallurgy, University of Chile ((Vaencia et al., 2004, 2006; Fuentes et al., 2002). They conducted numerical and experimental studies of the fluid dynamics in a Teniente-type copper converter. A three-dimensional simulation of the three-phase system was carried out using the volume of fluid (VOF) and the standard \( k - \varepsilon \) turbulence models implemented in a commercial solver. Their numerical model included the white metal and slag liquid phases, and gas phase through air injection from 50 submerged tuyeres, and experimental observations were carried out in a 1:5-scale water container. The results of these investigations enabled the operation conditions to be optimized. Royal (2007) also studied the flow characterization of Peirce-Smith copper converters. Although good results were obtained from the slice model, unfortunately it could not provide the entire flow field distribution of the furnace. Liow and Gray (1990) experimentally studied the formation of standing waves in a water model of a Peirce-Smith converter. The results showed that it was possible to obtain regions in the bath depth and tuyere angle/tuyere submergence plots where no standing waves were found and spitting was minimal. Kulkarni and Joshi (2005) presented a comprehensive review of bubble formation and bubble rise velocity in gas-liquid systems. In China, Professor Chi Mei and his group at Central South University (Li, Mei, and Zhang, 2001; Rao, 2010; Li, Chi, and Zhang, 2001; Chen, 2002; Mei et al., 2003) have focused mainly on the reaction kinetics, flow field, and industrial experiments on the copper flash smelting furnace.

* School of Metallurgical Science and Engineering, Central South University, China.
† Center for Innovation through Visualization and Simulation (CIVS), Purdue University Calumet, USA.
Numerical simulation of multiphase flow in a Vanyukov furnace

These studies have demonstrated that CFD and physical models are very effective ways to study the flow fields and other physical and chemical processes in these furnaces. However, there still remain many problems to be solved. A few papers have been published on heat and mass transfer inside the Vanyukov furnace. V.G. Lisienko presented a model to predict the behaviour of the furnace during emergency operation (Lisienko, 1995, Lisienko et al., 2012). Unfortunately, the multiphase flow features of the Vanyukov furnace, which could be critical for optimizing the actual operation and furnace design, have attracted little attention.

The objective of present work is to create a model that can predict the internal movement, the fluctuations, and the vortex formation in a Vanyukov furnace. The multiphase theories were first introduced, then an unsteady three-dimensional and three-phase flow model was built in ANSYS FLUENT® and calculated by using VOF and the k - ε model. The flow pattern, vortexes formation, and spectrum were thoroughly analysed, and finally the effects of air flow rates were calculated and analysed.

Methodology and theory
The flow inside the Vanyukov furnace is a typical complex multiphase flow. Currently, there are two approaches for the numerical calculation of multiphase flows: the Euler-Lagrange approach and the Euler-Euler approach. The latter was adopted in this work. In ANSYS FLUENT, three different Euler-Euler multiphase models are available: the VOF model, the mixture model, and the Eulerian model. The VOF model was used in the current investigation. The theories of VOF and the k - ε model are introduced in the following sections.

VOF model
The VOF formulation relies on the fact that two or more fluids (or phases) do not interpenetrate. If the ath volume fraction of fluid in the cell is denoted as VF, then the following three conditions are possible:

1. VF = 0: there is no fluid α in the cell
2.VF = 1: fluid α fills the cell
3.0 < VF < 1: the cell contains an interface between fluid α and one or more other fluids.

Tracking of the interface(s) between the phases is accomplished by the solution of a continuity equation for the volume fraction of one or more of the phases. For the ath phase, this equation has the following form:

\[ \frac{\partial}{\partial t} \left( r_\alpha \rho_\alpha \right) + \nabla \cdot (r_\alpha \rho_\alpha \vec{U}_\alpha) = S_\alpha + \sum_{\beta \neq \alpha} \left( m_{\alpha \beta} - m_{\beta \alpha} \right) \]

where \( r_\alpha \) is the volume fraction of phase α, \( \rho_\alpha \) is the density of phase α, \( \vec{U}_\alpha \) is the velocity of phase α, \( S_\alpha \) is the source term, \( m_{\alpha \beta} \) is the mass transfer from phase α to phase β, and \( m_{\beta \alpha} \) is the mass transfer from phase β to phase α.

In the VOF model, only a single momentum equation is accomplished by the solution of a continuity equation for the volume fraction of one or more of the phases. For the ath phase, the following equation has the following form:

\[ \rho = \sum_{\alpha} \rho_\alpha \]

\[ \mu = \sum_{\alpha} \mu_\alpha \]

\[ k = \sum_{\alpha} k_\alpha \]

\[ \varepsilon = \sum_{\alpha} \varepsilon_\alpha \]

where \( \rho \) is density, \( \vec{U} \) is velocity, \( \mu \) is viscosity, and \( F \) is force. For the three-phase system studied in this paper, the volume-fraction-averaged density and viscosity are calculated as follows:

\[ \rho = \frac{\sum_{\alpha} \rho_\alpha}{\sum_{\alpha} \rho_\alpha} \]

\[ \mu = \frac{\sum_{\alpha} \mu_\alpha}{\sum_{\alpha} \rho_\alpha} \]

\[ k = \frac{\sum_{\alpha} k_\alpha}{\sum_{\alpha} \rho_\alpha} \]

\[ \varepsilon = \frac{\sum_{\alpha} \varepsilon_\alpha}{\sum_{\alpha} \rho_\alpha} \]

k - ε model
The multiphase flow in the Vanyukov furnace should be solved with a fluid-dependent turbulence model. Due to its low computational cost and good numerical stability, the homogeneous k - ε turbulence model was applied in this study. The isotropic eddy viscosity (\( \mu_T \)) is characterized by the turbulence kinetic energy (\( k \)) and its dissipation rate (\( \varepsilon \)), which are given by:

\[ \frac{\partial}{\partial t} \left( \rho_k \right) + \nabla \cdot \left( \rho_k \vec{U} \right) = \nabla \cdot \left( \frac{G_k}{\sigma_k} \nabla k \right) + G_{k,\alpha} - \rho \varepsilon \]

\[ \frac{\partial}{\partial t} \left( \rho \varepsilon \right) + \nabla \cdot \left( \rho \vec{U} \varepsilon \right) = \nabla \cdot \left( \frac{\mu_T}{\sigma_\varepsilon} \nabla \varepsilon \right) + \frac{\varepsilon}{k} \left( C_1 \rho_k \varepsilon - C_2 \rho \varepsilon \right) \]

where, \( \rho_k \) and \( \vec{U} \) are the mixture density and velocity, respectively, \( \mu_T \) is the turbulent viscosity, \( G_k \) is the production of turbulence kinetic energy, and \( \sigma_k \) and \( \sigma_\varepsilon \) are the turbulent Prandtl numbers for \( k \) and \( \varepsilon \), respectively. The empirical constants appearing in the model are \( C_1 \) = 1.44, \( C_2 \) = 1.92, \( \sigma_k \) = 1.0, and \( \sigma_\varepsilon \) = 1.3.

Geometry and simulation conditions
Physical model
A typical hypothetical Vanyukov furnace (Figure 1) was created using information in the literature (Hongoi, 2001). There were 10 tuyeres on each side of the furnace to supply oxygen for the chemical reactions that take place in the slag layer. The tuyeres were located at the lower side of the furnace to ensure the high-speed enriched air could agitate the slag layer and provide enough oxygen for reaction inside the furnace.

The main dimension parameters of the furnace were as follows: total length 19 m, total width 2.5 m, height 6 m, exhaust gas tunnel height 9 m, tuyere height 2.5 m, slag layer depth 3.5 m, metal layer depth 0.9 m, metal output region length 2 m, and slag output region length 2 m.

As the objective of this work is to study the multiphase flow inside the furnace, the following simplifications were made:

- Heat and mass transfer were not considered
- The furnace structure was simplified, and could be modified according to the actual furnace dimensions
- Granular raw material feeding and liquid metal discharge were not considered.

CFD modelling
In order to carry out the CFD calculation, a multi-purpose geometry containing the fluid phases (exhaust gas, slag, and liquid metal) was created in Pre-Processor of ANSYS®. The geometry was then meshed with hexahedral elements. The
3D hexahedral mesh, as shown in Figure 1, consisted of approximately 500,000 elements. Since the structure of this Vanyukov furnace is composed of rectangular modules, it could be meshed with a hexahedral-structured mesh with an excellent fit.

After the mesh was generated, it was imported into ANSYS CFX® and then read into FLUENT®. The corresponding solver-type settings, material properties, boundary conditions, and operation conditions must be specified properly. The detail settings for FLUENT are shown in Table I. The boundary conditions and material properties are shown separately in Table II and Table III.

### Simulation procedure

Equations [1]–[6] were solved using the commercial solver Fluent 14.0. This package is a finite volume solver, using body-fitted grids. The pressure-velocity coupling was obtained using the SIMPLEC algorithm. For the time-dependent VOF and $k$-$\varepsilon$ calculations, the explicit time marching scheme with small time step $\Delta t = 1 \times 10^{-4}$ s was adopted. There were 443,264 control volumes, and the mesh was composed of hexahedral mesh elements. The computation of 6.6 seconds of operation of the furnace model consumed nearly 72 hours on a DELL® T7400 workstation with dual Xenon® CPUs (X5492, 3.4 GHz) and 16Gb memory running Windows® 7 Enterprise as operation system. This facility was provided by the Center for Innovation through Visualization and Simulation (CIVS) at Purdue University, Calumet in the USA.

### Results and discussion

The numerical simulation of this unsteady three-dimensional and three-phase flow can reveal many characteristics that cannot be measured or observed directly in a running furnace, such as the fluctuation of the slag surface in the injection zone, melt movements in the sedimentation region, and displacement of the slag layer to the sedimentation region. It is important to find the correct distribution of the flow field, so that the furnace can operate efficiently with proper inlet speed and with proper metal and slag height.

### Phase interface configuration

Distributions of the transient interfaces of three phases such as exhaust gas, metal, and slag at $t=6.62$ s are displayed in Figure 2. The 3D interfaces of overall slag-exhaust gas and slag-metal are presented in Figure 3, where the interface evolutions from $t=0.29$ s to $t=6.62$ s are listed separately.

### Table I

<table>
<thead>
<tr>
<th>FLUENT settings</th>
<th>Transient</th>
</tr>
</thead>
<tbody>
<tr>
<td>Solver type</td>
<td>VOF model</td>
</tr>
<tr>
<td>Multi-phase model</td>
<td>Standard k-$\varepsilon$ turbulent model</td>
</tr>
<tr>
<td>Turbulent model</td>
<td>1st-order upwind</td>
</tr>
<tr>
<td>Discretization scheme</td>
<td>Standard SIMPLE algorithm</td>
</tr>
</tbody>
</table>

### Table II

<table>
<thead>
<tr>
<th>Boundary conditions</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Enriched air flow rate, m.s$^{-1}$</td>
<td>70</td>
</tr>
<tr>
<td>Outlet pressure, Pa</td>
<td>-2000</td>
</tr>
<tr>
<td>Wall treatment</td>
<td>Standard wall functions</td>
</tr>
</tbody>
</table>

### Table III

<table>
<thead>
<tr>
<th>Material properties</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Metal density, kg.m$^{-3}$</td>
<td>5000</td>
</tr>
<tr>
<td>Metal viscosity, kg.m$^{-1}$.s$^{-1}$</td>
<td>0.004</td>
</tr>
<tr>
<td>Slag density, kg.m$^{-3}$</td>
<td>3000</td>
</tr>
<tr>
<td>Slag viscosity, kg.m$^{-1}$.s$^{-1}$</td>
<td>0.012</td>
</tr>
<tr>
<td>Exhaust gas density, kg.m$^{-3}$</td>
<td>1.29</td>
</tr>
<tr>
<td>Exhaust gas viscosity, kg.m$^{-1}$.s$^{-1}$</td>
<td>1.52 $\times$ 10$^{-5}$</td>
</tr>
</tbody>
</table>

Figure 2 – Contours of slag volume fraction at different axial positions when $t=6$ s: (a) $X=4.2$ m, (b) $Y=0.8$ m

Figure 1 – CFD model of Vanyukov furnace
Numerical simulation of multiphase flow in a Vanyukov furnace

The dynamic pressure of air injected into the furnace is much greater than the pressure head due to the depth of slag. Therefore, there is a blow-through distance, which is an air jet termed the ‘gas jet core’ that initially enters the liquid, and bubbles are created in the molten slag as shown in Figure 3(a) to Figure 3(c). As the air bubbles impinge the slag intermittently, the wave at the interface of slag-metal and exhaust gas-slag is formed as a result of horizontal jet and upwelling flow in the air injection. The configuration of the slag surface at the interface between slag and exhaust gas is displayed in Figure 3, where the spout peak of combined flow can be observed. The slag becomes more active above the tuyere position, while it is more quiescent under it. As the flows are unsteady, the configurations of the phase interface are transient phenomena. The interface between the slag and metal is very quiescent, which is beneficial for metal.

Figure 3 – Contours for slag volume fraction of 0.5 in different time steps: (a) \(t=0.29\) s; (b) \(t=0.55\) s; (c) \(t=0.95\) s; (d) \(t=2.15\) s; (e) \(t=2.95\) s; (f) \(t=4.15\) s; (g) \(t=4.95\) s; (h) \(t=6.62\) s
separation. It is very important that with this flow field distribution, the chemical reaction can proceed to completion in the injection region, while the metal can settle in the sediment region with no stirring.

**Velocity field distribution**

The velocity vectors and contours at the main section for all zones, including air, metal, and slag phases, are shown in Figures 4, 5, and 6 respectively.

The flow pattern is in accordance with previous results (Hongjiu, 2001). Nevertheless, the flow pattern near the slag layer is very complex and unstable, and some vortices are observed. Variations in flow patterns are caused by the differences in physical properties of slag, air, and metal.

The enriched air injected from the tuyere into the slag layer could stir the slag layer and accelerate the chemical reaction. The transient maximum values of exhaust gas, slag, and metal are 22.894 m/s, 70.00 m/s, and 0.0555 m/s respectively. Figures 4(f), 5, 6(c), and 6(d) show that the velocity in the slag settling region is very low. This could be due to the separate wall blocking the vigorous stirring in the injection region. The same phenomenon can also be found in the metal settling region. Therefore, by using this model, the height, spatial position, and thickness of the separate wall can be optimized to obtain the best flow pattern in the settling regions.

The oxygen-enriched air also causes the vortex movement and fluctuation. The air will push the slag towards the centre of the furnace and the upper interface. Several small vortices can be found in slag region, as shown in Figure 5. It is apparent that the velocity would be significantly reduced away from the tuyere zone. This is because of the huge density difference between the slag and enriched air (nearly 300). From this point of view, the model can also be used to optimize the tuyere structure and its operational configurations, such as tuyere diameter, tuyere angle, number and arrangement of tuyeres, and air flow rates.

**Air flow distribution**

Figure 7 depicts the path lines of the enriched air. Most of the air is injected directly into the slag layer and escapes from the slag-exhaust gas interface in the area located at nearly one-quarter of the width. This indicates that the current air speed (or tuyere pressure) and tuyere configuration is not good enough for the air to penetrate through the slag layer. The air flow above the slag is turbulent, which can be an important basis for determining the granular raw material distribution.

**Spectrum analysis**

Wave formation at the slag/exhaust duct interface is another important factor for slag emulsification. It is known that as the wave fluctuation becomes stronger, the slag layer becomes easier to break up and be mixed with the granular raw material. The fluctuation of density with time and power density spectrum with frequency at the selected point P1 (X=4 m, Y=0.8 m, Z=2.2 m) are shown in Figures 8 and 9 respectively. The fluctuation of density indicates that at this point the two phases (slag and air) are present in different instants. The density first drops to nearly zero in 0.3
Numerical simulation of multiphase flow in a Vanyukov furnace

seconds, then increases to 3000 kg/m³ and begins oscillating between 1500 kg/m³ and 3000 kg/m³. This indicates that the enriched air injected into the slag layer at first creates a hollow near the tuyere area, and then, as shown in Figure 3, stirs the slag layer vigorously. From the fast Fourier transform (FFT) of this density signal, we obtain the dominant frequency of the density variation, $\omega = 0.29$ Hz, as shown in Figure 9.

Effect of air flow rate
Since the viscosity of the slag and the interface tension between slag and air are large, a large momentum is needed for air to overcome the interface tension and viscous force in the slag layer. This strong flow, which is directed horizontally initially and then upward and sideways, may drag the slag into the air flow, resulting in vigorous emulsification. Consequently, the effect of air flow rate is of interest. Using
The injection flow rate of argon gas has a major effect on the mean slag velocity. The peak mean velocity increases from 2.17 m/s to 4.99 m/s as the flow rate of enriched air increases from 70 m/s to 160 m/s. A higher efficiency of desulphurization can be achieved at higher air flow rates.

The proposed model provides a method to optimize furnace structural and operational conditions, such as the number of tuyeres, the angle of injection, the heights of the slag and metal layers, the dimension of the furnace, and the inlet of granular raw material.

Acknowledgement
The authors would like to thank the Center for Innovation through Visualization and Simulation at Purdue University for offering this research opportunity and for assistance during the course of this work. The authors are also grateful for the financial support of the National Natural Science Foundation of China (51274241, 61321003).

References


INTERNATIONAL ACTIVITIES

2015

14–17 June 2015 — European Metallurgical Conference
Dusseldorf, Germany
Website: http://www.emc.gdmb.de

Dusseldorf, Germany
Website: http://www.pb-zn.gdmb.de

Dusseldorf, Germany
Website: http://www.metec-tradefair.com

6–8 July 2015 — Copper Cobalt Africa Incorporating The 8th Southern African Base Metals Conference
Zambezi Sun Hotel, Victoria Falls, Livingstone, Zambia
Contact: Raymond van der Berg
Tel: +27 11 834-1273/7
Fax: +27 11 838-5923/833-8156
E-mail: raymond@saimm.co.za
Website: http://www.saimm.co.za

15–16 July 2015 — Virtual Reality and spatial information applications in the mining industry Conference 2015
University of Pretoria
Contact: Camielah Jardine
Tel: +27 11 834-1273/7
Fax: +27 11 838-5923/833-8156
E-mail: camielah@saimm.co.za
Website: http://www.saimm.co.za

Vineyard Hotel, Newlands, Cape Town
Contact: Raymond van der Berg
Tel: +27 11 834-1273/7
Fax: +27 11 838-5923/833-8156
E-mail: raymond@saimm.co.za
Website: http://www.saimm.co.za

19–20 August 2015 — The Danie Krige Geostatistical Conference: Geostatistical geovalue — rewards and returns for spatial modelling
Crown Plaza, Johannesburg
Contact: Yolanda Ramokgadi
Tel: +27 11 834-1273/7
Fax: +27 11 838-5923/833-8156
E-mail: yolanda@saimm.co.za
Website: http://www.saimm.co.za

25–27 August 2015 — Coal Processing – Unlocking Southern Africa's Coal Potential
Graceland Hotel Casino and Country Club Secunda
Contact: Ann Robertson
Tel: +27 11 433-0063

26–28 August 2015 — MINESafe 2015—Sustaining Zero Harm: Technical Conference and Industry day
Emperors Palace Hotel Casino, Convention Resort, Johannesburg
Contact: Raymond van der Berg
Tel: +27 11 834-1273/7
Fax: +27 11 838-5923/833-8156
E-mail: raymond@saimm.co.za,
Website: http://www.saimm.co.za

28 September-2 October 2015 — WorldGold Conference 2015
Misty Hills Country Hotel and Conference Centre, Cradle of Humankind, Gauteng, South Africa
Contact: Camielah Jardine
Tel: +27 11 834-1273/7
Fax: +27 11 838-5923/833-8156,
E-mail: camielah@saimm.co.za
Website: http://www.saimm.co.za

12–14 October 2015 — Slope Stability 2015: International Symposium on slope stability in open pit mining and civil engineering
In association with the Surface Blasting School
15–16 October 2015
Cape Town Convention Centre, Cape Town
Contact: Raymond van der Berg
Tel: +27 11 834-1273/7
Fax: +27 11 838-5923/833-8156
E-mail: raymond@saimm.co.za
Website: http://www.saimm.co.za

20 October 2015 — 13th Annual Southern African Student Colloquium
Mintek, Randburg, Johannesburg
Contact: Yolanda Ramokgadi
Tel: +27 11 834-1273/7
Fax: +27 11 838-5923/833-8156
E-mail: yolanda@saimm.co.za
Website: http://www.saimm.co.za
INTERNATIONAL ACTIVITIES

21–22 October 2015 — Young Professionals 2015 Conference
Making your own way in the minerals industry
Mintek, Randburg, Johannesburg
Contact: Camielah Jardine
Tel: +27 11 834-1273/7
Fax: +27 11 838-5923/833-8156
E-mail: camielah@saimm.co.za
Website: http://www.saimm.co.za

28–30 October 2015 — AMI: Nuclear Materials Development Network Conference
Nelson Mandela Metropolitan University, North Campus Conference Centre, Port Elizabeth
Contact: Raymond van der Berg
Tel: +27 11 834-1273/7
Fax: +27 11 838-5923/833-8156
E-mail: raymond@saimm.co.za
Website: http://www.saimm.co.za

8–13 November 2015 — MPES 2015: Twenty Third International Symposium on Mine Planning & Equipment Selection
Sandton Convention Centre, Johannesburg, South Africa
Contact: Raj Singhal
E-mail: singhal@shaw.ca or E-mail: raymond@saimm.co.za
Website: http://www.saimm.co.za

17–18 May 2016 — The SAMREC/SAMVAL Companion Volume Conference
Johannesburg
Contact: Yolanda Ramokgadi
Tel: +27 11 834-1273/7
Fax: +27 11 838-5923/833-8156
E-mail: yolanda@saimm.co.za
Website: http://www.saimm.co.za

May 2016 — PASTE 2016 International Seminar on Paste and Thickened Tailings
Kwa-Zulu Natal, South Africa
Contact: Raymond van der Berg
Tel: +27 11 834-1273/7
Fax: +27 11 838-5923/833-8156
E-mail: raymond@saimm.co.za
Website: http://www.saimm.co.za

9–10 June 2016 — 1st International Conference on Solids Handling and Processing A Mineral Processing Perspective
South Africa
Contact: Raymond van der Berg
Tel: +27 11 834-1273/7
Fax: +27 11 838-5923/833-8156
E-mail: raymond@saimm.co.za
Website: http://www.saimm.co.za

1–3 August 2016 — Hydrometallurgy Conference 2016
‘Sustainability and the Environment’ in collaboration with MinProc and the Western Cape Branch
Cape Town
Contact: Raymond van der Berg
Tel: +27 11 834-1273/7
Fax: +27 11 838-5923/833-8156
E-mail: raymond@saimm.co.za
Website: http://www.saimm.co.za

16–19 August 2016 — The Tenth International Heavy Minerals Conference ‘Expanding the horizon’
Sun City, South Africa
Contact: Camielah Jardine
Tel: +27 11 834-1273/7
Fax: +27 11 838-5923/833-8156
E-mail: camielah@saimm.co.za
Website: http://www.saimm.co.za
## Company Affiliates

The following organizations have been admitted to the Institute as Company Affiliates:

<table>
<thead>
<tr>
<th>Company Name</th>
</tr>
</thead>
<tbody>
<tr>
<td>AECOM SA (Pty) Ltd</td>
</tr>
<tr>
<td>AEL Mining Services Limited</td>
</tr>
<tr>
<td>Air Liquide (PTY) Ltd</td>
</tr>
<tr>
<td>AMEC Mining and Metals</td>
</tr>
<tr>
<td>AMIRA International Africa (Pty) Ltd</td>
</tr>
<tr>
<td>ANDRITZ Delkor (Pty) Ltd</td>
</tr>
<tr>
<td>Anglo Operations Ltd</td>
</tr>
<tr>
<td>Anglo Platinum Management Services (Pty) Ltd</td>
</tr>
<tr>
<td>Anglogold Ashanti Ltd</td>
</tr>
<tr>
<td>Atlas Copco Holdings South Africa (Pty) Limited</td>
</tr>
<tr>
<td>Aurecon South Africa (Pty) Ltd</td>
</tr>
<tr>
<td>Aveng Moolmans (Pty) Ltd</td>
</tr>
<tr>
<td>Axis House (Pty) Ltd</td>
</tr>
<tr>
<td>Bafokeng Rasimone Platinum Mine</td>
</tr>
<tr>
<td>Barloworld Equipment - Mining</td>
</tr>
<tr>
<td>BASF Holdings SA (Pty) Ltd</td>
</tr>
<tr>
<td>Bateman Minerals and Metals (Pty) Ltd</td>
</tr>
<tr>
<td>BCL Limited</td>
</tr>
<tr>
<td>Becker Mining (Pty) Ltd</td>
</tr>
<tr>
<td>BedRock Mining Support (Pty) Ltd</td>
</tr>
<tr>
<td>Bell Equipment Company (Pty) Ltd</td>
</tr>
<tr>
<td>BHP Billiton Energy Coal SA Ltd</td>
</tr>
<tr>
<td>Blue Cube Systems (Pty) Ltd</td>
</tr>
<tr>
<td>Bluhm Burton Engineering (Pty) Ltd</td>
</tr>
<tr>
<td>Blyvooruitzicht Gold Mining Company Ltd</td>
</tr>
<tr>
<td>BSC Resources</td>
</tr>
<tr>
<td>CAE Mining (Pty) Limited</td>
</tr>
<tr>
<td>Caledonia Mining Corporation</td>
</tr>
<tr>
<td>CDM Group</td>
</tr>
<tr>
<td>CGG Services SA</td>
</tr>
<tr>
<td>Chamber of Mines</td>
</tr>
<tr>
<td>Concor Mining</td>
</tr>
<tr>
<td>Concor Technicrete</td>
</tr>
<tr>
<td>Council for Geoscience Library</td>
</tr>
<tr>
<td>CSIR–Natural Resources and the Environment</td>
</tr>
<tr>
<td>Department of Water Affairs and Forestry</td>
</tr>
<tr>
<td>Deutsche Securities (Pty) Ltd</td>
</tr>
<tr>
<td>Digby Wells and Associates</td>
</tr>
<tr>
<td>Downer EDI Mining</td>
</tr>
<tr>
<td>DRA Mineral Projects (Pty) Ltd</td>
</tr>
<tr>
<td>DTP Mining</td>
</tr>
<tr>
<td>Duraset</td>
</tr>
<tr>
<td>Elbroc Mining Products (Pty) Ltd</td>
</tr>
<tr>
<td>Engineering and Project Company Ltd</td>
</tr>
<tr>
<td>eThekweni Municipality</td>
</tr>
<tr>
<td>Exxaro Coal (Pty) Ltd</td>
</tr>
<tr>
<td>Exxaro Resources Limited</td>
</tr>
<tr>
<td>Fasken Martineau</td>
</tr>
<tr>
<td>FLSmidth Minerals (Pty) Ltd</td>
</tr>
<tr>
<td>Fluor Daniel SA (Pty) Ltd</td>
</tr>
<tr>
<td>Franki Africa (Pty) Ltd</td>
</tr>
<tr>
<td>Johannesburg</td>
</tr>
<tr>
<td>Fraser Alexander Group</td>
</tr>
<tr>
<td>Glencore</td>
</tr>
<tr>
<td>Goba (Pty) Ltd</td>
</tr>
<tr>
<td>Hall Core Drilling (Pty) Ltd</td>
</tr>
<tr>
<td>Hatch (Pty) Ltd</td>
</tr>
<tr>
<td>Herrenknecht AG</td>
</tr>
<tr>
<td>HPE Hydro Power Equipment (Pty) Ltd</td>
</tr>
<tr>
<td>Impala Platinum Limited</td>
</tr>
<tr>
<td>IMS Engineering (Pty) Ltd</td>
</tr>
<tr>
<td>JENNMAR South Africa</td>
</tr>
<tr>
<td>Joy Global Inc. (Africa)</td>
</tr>
<tr>
<td>Leco Africa (Pty) Limited</td>
</tr>
<tr>
<td>Longyear South Africa (Pty) Ltd</td>
</tr>
<tr>
<td>Lonmin Plc</td>
</tr>
<tr>
<td>Ludowici Africa</td>
</tr>
<tr>
<td>Lull Storm Trading (PTY)Ltd T/A Wekaba Engineering</td>
</tr>
<tr>
<td>Magnetech (Pty) Ltd</td>
</tr>
<tr>
<td>Magotteaux(PTY) LTD</td>
</tr>
<tr>
<td>MBE Minerals SA Pty Ltd</td>
</tr>
<tr>
<td>MCC Contracts (Pty) Ltd</td>
</tr>
<tr>
<td>MDM Technical Africa (Pty) Ltd</td>
</tr>
<tr>
<td>Metalock Industrial Services Africa (Pty)Ltd</td>
</tr>
<tr>
<td>Metorex Limited</td>
</tr>
<tr>
<td>Metso Minerals (South Africa) (Pty) Ltd</td>
</tr>
<tr>
<td>Minerals Operations Executive (Pty) Ltd</td>
</tr>
<tr>
<td>MineRP Holding (Pty) Ltd</td>
</tr>
<tr>
<td>Mintek</td>
</tr>
<tr>
<td>MIP Process Technologies</td>
</tr>
<tr>
<td>Modular Mining Systems Africa (Pty) Ltd</td>
</tr>
<tr>
<td>MSA Group (Pty) Ltd</td>
</tr>
<tr>
<td>Multotec (Pty) Ltd</td>
</tr>
<tr>
<td>Murray and Roberts Cementation</td>
</tr>
<tr>
<td>Nalco Africa (Pty) Ltd</td>
</tr>
<tr>
<td>Namakwa Sands (Pty) Ltd</td>
</tr>
<tr>
<td>New Concept Mining (Pty) Limited</td>
</tr>
<tr>
<td>Northam Platinum Ltd - Zondereinde</td>
</tr>
<tr>
<td>Osborn Engineered Products SA (Pty) Ltd</td>
</tr>
<tr>
<td>Outotec (RSA) (Proprietary) Limited</td>
</tr>
<tr>
<td>PANalytical (Pty) Ltd</td>
</tr>
<tr>
<td>Paterson and Cooke Consulting Engineers (Pty) Ltd</td>
</tr>
<tr>
<td>Polysius A Division of Thyssenkrupp Industrial Solutions (Pty) Ltd</td>
</tr>
<tr>
<td>Precious Metals Refiners</td>
</tr>
<tr>
<td>Rand Refinery Limited</td>
</tr>
<tr>
<td>Redpath Mining (South Africa) (Pty) Ltd</td>
</tr>
<tr>
<td>Rosond (Pty) Ltd</td>
</tr>
<tr>
<td>Royal Bafokeng Platinum</td>
</tr>
<tr>
<td>Roytek Technoloogies (Pty) Ltd</td>
</tr>
<tr>
<td>Runge Pinco Minauro Limited</td>
</tr>
<tr>
<td>Rustenberg Platinum Mines Limited</td>
</tr>
<tr>
<td>SAIEG</td>
</tr>
<tr>
<td>Salene Mining (Pty) Ltd</td>
</tr>
<tr>
<td>Sandvik Mining and Construction Delmas (Pty) Ltd</td>
</tr>
<tr>
<td>Sandvik Mining and Construction RSA(Pty) Ltd</td>
</tr>
<tr>
<td>SANIRE</td>
</tr>
<tr>
<td>Sasol Mining(Pty) Ltd</td>
</tr>
<tr>
<td>Scannin Africa (Pty) Ltd</td>
</tr>
<tr>
<td>Sebilo Resources (Pty) Ltd</td>
</tr>
<tr>
<td>SENET</td>
</tr>
<tr>
<td>Senmin International (Pty) Ltd</td>
</tr>
<tr>
<td>Shaft Sinkers (Pty) Limited</td>
</tr>
<tr>
<td>Sibanye Gold (Pty) Ltd</td>
</tr>
<tr>
<td>Smec SA</td>
</tr>
<tr>
<td>SMS Siemag South Africa (Pty) Ltd</td>
</tr>
<tr>
<td>SNC Lavalin (Pty) Ltd</td>
</tr>
<tr>
<td>Sound Mining Solutions (Pty) Ltd</td>
</tr>
<tr>
<td>SRK Consulting SA (Pty) Ltd</td>
</tr>
<tr>
<td>Technology Innovation Agency</td>
</tr>
<tr>
<td>Time Mining and Processing (Pty) Ltd</td>
</tr>
<tr>
<td>Tomra Sorting Solutions Mining (Pty) Ltd</td>
</tr>
<tr>
<td>TWP Projects (Pty) Ltd</td>
</tr>
<tr>
<td>Ukwazi Mining Solutions (Pty) Ltd</td>
</tr>
<tr>
<td>Umgeni Water</td>
</tr>
<tr>
<td>VBKOM Consulting Engineers</td>
</tr>
<tr>
<td>Webber Wentzel</td>
</tr>
<tr>
<td>Weir Minerals Africa</td>
</tr>
</tbody>
</table>
For the past 120 years, the Southern African Institute of Mining and Metallurgy, has promoted technical excellence in the minerals industry. We strive to continuously stay at the cutting edge of new developments in the mining and metallurgy industry. The SAIMM acts as the corporate voice for the mining and metallurgy industry in the South African economy. We actively encourage contact and networking between members and the strengthening of ties. The SAIMM offers a variety of conferences that are designed to bring you technical knowledge and information of interest for the good of the industry. Here is a glimpse of the events we have lined up for 2015. Visit our website for more information.

Website: http://www.saimm.co.za
Applying Poka Yokes in the mining industry

Pre-stressing Units
Areal Coverage
Roofbolts
Monitoring Devices
Accessories

New Concept Mining
Integrated systems of support

© New Concept Mining 2015
www.ncm.co.za
+27 11 494 6000
Patents Pending