Pyrometallurgical Modelling Principles and Practices

Workshop

5 August 2014
Emperors Palace Hotel Casino Convention Resort, Johannesburg
Workshop Programme

Day 2—Tuesday, 5 August 2014 (Workshop)

07:30—08:00 Registration & Early Morning Refreshments

08:00—08:10 Venue Safety Presentation

08:10—08:20 Welcome: Conference Chair

Workshop Presenters

Prof. Chris Pistorius
Dr Johan Zietsman

08:20—10:30 Introduction to mathematical modelling
• Mathematical modelling background
• Modelling and simulation practice
• Process modelling fundamentals

10:30—11:00 Morning Tea

11:00—12:30 Pyrometallurgical process balances: principles
• Stoichiometry; enthalpy; structuring the process balance
• Examples: combustion of gaseous fuel, including departure from equilibrium

12:30—13:30 Lunch

13:30—15:00 Pyrometallurgical process balances: nonideal solutions and kinetics
• Combustion examples: coal
• Heat of solution and heat of reaction: aluminium deoxidation; slag enthalpy
• Mass balances in simple reaction kinetics

15:00—15:30 Afternoon Tea

15:30—17:00 Techno-economic modelling
• Simple cost examples
• A process model as part of a broader project financial model
Workshop Presenters

Prof. C Pistorius

Chris Pistorius is the POSCO Professor of Iron and Steelmaking in the Department of Materials Science and Engineering at Carnegie Mellon University (Pittsburgh, PA, USA), where he has been since 2008. Previously he was Professor and Head of Department of Materials Science and Metallurgical Engineering at the University of Pretoria. He holds Bachelor’s and Master’s degrees in Metallurgical Engineering from the University of Pretoria, and a PhD from the University of Cambridge, United Kingdom. His current research interests include the fundamentals of ironmaking and steelmaking reactions, and electrochemistry of corrosion and metals production.

Dr Johan Zietsman

Johan Zietsman is the GlencoreXstrata Chair in Pyrometallurgical Modelling in the Department of Materials Science and Metallurgical Engineering at the University of Pretoria since February 2013. Previously he was founder and managing director of Ex Mente Technologies, a metallurgical engineering systems and consulting firm. He holds a Bachelor, Master’s and Ph.D. degree from the University of Pretoria, South Africa. His current research interests include modelling of material properties, lumped parameter modelling of metallurgical processes, thermochemical analysis, multiphysics modelling and techno-economic modelling of metallurgical operations.
Introduction to Mathematical Modelling
Mathematical Modelling – Introduction
"Models have limitations; stupidity does not!!"
Prof. Michael Athans, MIT
Lecture Purpose

- Provide some background on mathematical modelling.
- Present some useful principles and practices for modelling and simulation.
- Present some fundamentals of process modelling.
Mathematical Modelling – background
Table of contents

1. Basic Concepts
   - Terminology
   - Motivation

2. Classification of Mathematical Models
   - Phenomenological vs. Empirical
   - Distributed Parameter vs. Lumped Parameter
   - Macroscopic vs. Microscopic
“Programming today is a race between software engineers striving to build bigger and better idiot-proof programs, and the universe trying to produce bigger and better idiots. So far, the universe is winning.”

Richard Cook, comedian
<table>
<thead>
<tr>
<th>Terminology</th>
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<tbody>
<tr>
<td><strong>model</strong></td>
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<tr>
<td>&quot;...something that mimics relevant features of the situation being studied.&quot; (Bender 1978)</td>
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<tr>
<td><strong>mathematical model</strong></td>
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<td>&quot;... an abstract, simplified, mathematical construct related to a part of reality and created for a particular purpose.&quot; (Bender 1978)</td>
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<tr>
<td>&quot;... a mathematical construct designed to study a particular real-world system or phenomenon.&quot; (Giordano and Weir 1985)</td>
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<tr>
<td><strong>mathematical modelling</strong></td>
</tr>
<tr>
<td>The process of creating a mathematical model.</td>
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<tr>
<td><strong>simulation</strong></td>
</tr>
<tr>
<td>The process of using mathematical models to simulate real-world systems being studied.</td>
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</table>
Three reasons why you would build and use mathematical model?

Three reasons why you would NOT build and use mathematical model?

What alternatives are there to mathematical modelling?
Why use modelling in metallurgical engineering?

- Sometimes it is the only feasible way.  
  (Simulating nuclear war.)
- Measurement techniques may not allow direct observation.  
  (Temperature distribution in the slag bath of a smelter.)
- It may be cheaper.
- It may be faster.  
  (Model versus pilot plant.)
- It is part of a combined approach.  
  (Measure and model.)
Why use modelling in metallurgical engineering?

Useful in all stages of process engineering:
- Education
- R&D
- Conceptualisation
- Feasibility study
- Design
- Plant operation
- Plant optimisation
Why NOT model?

- The mathematics may be too complex.
- The problem may be too large to solve.
- The knowledge and skills may not be available.
Alternatives to mathematical modelling?

- Laboratory experiments.
- Pilot plant experiments.
- Industrial experiments and measurements.
Phenomenological vs. Empirical

- Phenomenological (white box): Explicitly describe the phenomena of interest using mathematics. (E.g. CFD models, mass and energy balances)
- Empirical (black box): Implicitly describe the phenomena of interest based on collected data, data processing algorithms and information derived from these.
- Combined (grey box): Very few completely phenomenological models are used in our field. In most cases some empirically derived data are required.

This course focuses on a largely phenomenological approach to modelling processes, while including empirical components where necessary.
Distributed Parameter vs. Lumped Parameter

- Distributed parameter models: The domain is broken up into small elements and dependent variables are calculated for each element. (E.g. finite element method, finite volume method, finite difference method, discrete element method.)
- Lumped parameter models: The domain is not broken up, or is broken up into large regions. Dependent variables are calculated for the system as a whole, or for each region. (E.g. mass and energy balances, flowsheet type models)

This course focuses on lumped parameter models for the first two blocks. Thereafter the discrete element method will be studied. Microscopic vs. macroscopic
Macroscopic vs. Microscopic

- Macroscopic models:
  These models usually focus on large real-world systems, and describe phenomena at a macroscopic level. (E.g. Heat transfer, fluid flow, mass and energy balancing, etc.)

- Microscopic models:
  These models attempt to describe the very basic behaviour of materials and small systems by using atomic-level principles. (E.g. quantum mechanical models, thermochemical solution models, viscosity models, etc.)

This course focuses on macroscopic models of processes and process flow sheets.
Pyrometallurgical Modelling *Principles and Practices*

Literature

- Bender 1978
- Giordano and Weir 1985
Mathematical Modelling and Simulation – principles and practices
"Model building involves imagination and skill. Giving rules for doing it is like listing rules for being an artist: at best this provides a framework around which to build skills and develop imagination."

(Bender 1978)
# Table of contents

1. Overview
   - Motivation

2. Principles
   - Python
   - Modelling and Simulation

3. Practices
   - Modelling
   - Simulation
   - Documentation
Why are principles and practices important?
Importance of Principles and Practices

Modelling is sometimes viewed as a quick and easy way of getting answers. Sometimes it is. But what do the answers mean? Can we really trust them? Can we make decisions involving thousands or millions of dollars based on our answers? Can we build and modify equipment and plants based on our modelling results? Can we risk people’s lives based on them?
We need to be able to apply modelling and simulation

- responsibly,
- effectively, and
- reliably;
otherwise you may as well be playing computer games.
The Zen of Python

Beautiful is better than ugly.
Explicit is better than implicit.
Simple is better than complex.
Complex is better than complicated.
Flat is better than nested.
Sparse is better than dense.
Readability counts.
Special cases aren’t special
enough to break the rules.
Although practicality beats
purity.
Errors should never pass silently.
Unless explicitly silenced.

In the face of ambiguity, refuse the
temptation to guess.
There should be one— and preferably
only one —obvious way to do it.
Although that way may not be obvious
at first unless you’re Dutch.
Now is better than never.
Although never is often better than
right now.
If the implementation is hard to explain,
it’s a bad idea.
If the implementation is easy to explain,
it may be a good idea.
Namespaces are one honking great idea
— let’s do more of those!

Julian Simon
SAIMM Pyrometallurgical Modelling Workshop 2013
Modelling and Simulation Principles

- Competent is better than incompetent.
- Showing is better than hiding.
- Beautiful is better than ugly.
- Clear is better than vague.
- Explicit is better than implicit.
- Simple is better than complex.
- Complex is better than complicated.
- Together is better than alone.
- Now is better than never.
- Although never is often better than right now.
What process should we follow to develop a mathematical model in an effective, responsible and reliable way?
The Modelling Process

- Problem definition
- Requirement specification
- System analysis
- Formulation
- Implementation
- Verification
- Validation
- Acceptance
- Release
- Communicate
- Use

"V" model of software development.
Pyrometallurgical Modelling *Principles and Practices*

Mathematical Modelling Process

Problem Definition

- Clearly define your problem.
- Often difficult.
- Takes time to develop an appreciation.
- Very important. It determines your direction.

- Problem definition
- Requirement specification
- System analysis
- Formulation
- Implementation
- Verification
- Validation
- Acceptance
- Release
- Communicate
- Use

Aiden Zimmermann  SAIMM Pyrometallurgical Modelling Workshop 2019
Mathematical Modelling Process

Requirement Specification

1. Define the system scope.
2. Specify the required results.
3. How important is validation.
4. Specify acceptance criteria.
5. This will help you to focus on a finite task.

- Problem definition
- Requirement specification
- System analysis
- Formulation
- Implementation
- Verification
- Validation
- Acceptance
- Release
- Communicate
- Use

Adrian Zimmeri  SAIMM Pyrometallurgical Modelling Workshop 2014
Mathematical Modelling Process

System Analysis

- Clearly describe your system.
- Clearly describe all materials.
- Identify key phenomena.
- Think about how you will do validation.

System analysis
- Formulation
- Implementation
- Verification
- Validation
- Acceptance
- Release
- Communicate
- Use
Mathematical Modelling Process

Formulation

- Describe your modelling approach.
- Overview your model.
- Provide explicit details of the model.
- Specify verification and validation requirements.
- See model manual template.
- Formulation must allow implementation.

- Problem definition
- Requirement specification
- System analysis
- Formulation
- Implementation
- Verification
- Validation
- Acceptance
- Release
- Communicate
- Use

Adrian Ziman
SAIMM Pyrometallurgical Modelling Workshop 2014
Mathematical Modelling Process

Implementation

- Describe implementation approach.
- Provide explicit details of the implementation.
- Specify verification and validation requirements.
- See model manual template.
- Formulation must allow co-development.

- Problem definition
- Requirement specification
- System analysis
- Formulation
- Implementation
- Verification
- Validation
- Acceptance
- Release
- Communicate
- Use

Johan Zanzani  SAIMM Pyrometallurgical Modelling Workshop 2013
Mathematical Modelling Process

- Problem definition
- Requirement specification
- System analysis
- Formulation
- Implementation
- Verification
- Validation
- Acceptance
- Release
- Communicate
- Use

- Confirm sound formulation and implementation.
- Describe implementation approach.
- Summarise verification criteria.
- Provide details of tests and results.
- See model manual template.

Adam Zeman | SAIMM Pyrometallurgical Modelling Workshop 2014
Mathematical Modelling Process

Validation

- Confirm valid description of actual system.
- Describe implementation approach.
- Summarise validation criteria.
- Provide details of tests and results.
- See model manual template.

- Problem definition
- Requirement specification
- System analysis
- Formulation
- Implementation
- Verification
- Validation
- Acceptance
- Release
- Communicate
- Use

Adrian Zeman
SAIMM Pyrometallurgical Modelling Workshop 2014
Pyrometallurgical Modelling *Principles and Practices*

Mathematical Modelling Process

- Confirm that the model fulfills the stated requirement.
- Describe acceptance approach.
- Summarize acceptance criteria.
- Provide details of tests and results.
- See model manual template.

- Problem definition
- Requirement specification
- System analysis
- Formulation
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- Use

Author: Ziman
SAIMM Pyrometallurgical Modelling Workshop 2018
Pyrometallurgical Modelling *Principles and Practices*

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**Mathematical Modelling Process**

- Make sure all documentation and code are up to date.
- Package the current model manual and software as formal revision.
- Provide user instructions. Especially capabilities and limitations.
- See model manual template.
- Problem definition
- Requirement specification
- System analysis
- Formulation
- Implementation
- Verification
- Validation
- Acceptance
- Release
- Communicate
- Use

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Mathematical Modelling Process

- Problem definition
- Requirement specification
- System analysis
- Formulation
- Implementation
- Verification
- Validation
- Acceptance
- Release
- Communicate
- Use

Inform all relevant persons of the release.

Explain/present important changes and updates clearly.

Adam Zeman
SAIMM Pyrometallurgical Modelling Workshop 2011
Now we are ready to use the model in investigations.
What process should we follow to perform a simulation investigation in an effective, responsible and reliable way?
Simulation Investigation Process

1. Purpose statement
2. Requirement specification
3. Plan investigation
4. Collect required data
5. Execute scenarios
6. Analyse and interpret scenario results
7. Analyse and interpret investigation results
8. Communicate results
Simulation Investigation Process

Requirement Specification

- Clearly define the scope of the investigation.
- Specify the results that you need to produce.
- This will focus you on a finite task.

1. Purpose statement
2. Requirement specification
3. Plan investigation
4. Collect required data
5. Execute scenarios
6. Analyze and interpret scenario results
7. Analyze and interpret investigation results
8. Communicate results
Important Documentation Aspects

- References:
  - Documents (articles, reports, etc.)
  - Sources of data (be very clear and specific)
- Nomenclature:
  - List of terms (glossary)
  - List of symbols
  - List of subscripts
  - List of acronyms and abbreviations
- Units of measure
Literature used in this lecture:

- Bender 1979
- Giordano and Weir 1985
- Oberkampf and Trucano 2002
- Zietsman 2004
<table>
<thead>
<tr>
<th>Principles</th>
<th>Practice</th>
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<tr>
<td>Modelling</td>
<td>Simulation</td>
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<tr>
<td>Documentation</td>
<td></td>
</tr>
</tbody>
</table>

Adam Zeman  SAIMM Pyrometallurgical Modelling Workshop 2011
Mathematical Modelling – process modelling fundamentals
### Table of Contents

1. Fundamental Laws
   - Mass Conservation
   - Energy Conservation
   - Others
Mass Balance Equation

Complete form: \( \frac{dt_j}{dt} = \sum_{i=1}^{n_i} m_{in,i} - \sum_{i=1}^{n_{ag}} m_{out,j} \)

Steady state form: \( \sum_{i=1}^{n_{in}} m_{in,i} = \sum_{i=1}^{n_{out}} m_{out,j} \)

- Based on the principle of mass conservation.
Element Balance Equations

For element $j$:

Complete form:  
$$\frac{dm_j}{dt} = \sum_{i=1}^{n} m_{j,\text{in},i} - \sum_{i=1}^{n} m_{j,\text{out},i}$$

Steady state form:  
$$\sum_{i=1}^{n} m_{j,\text{in},i} = \sum_{i=1}^{n} m_{j,\text{out},i}$$

- Based on the principle of mass conservation.
- An important verification tool for modelling chemically reactive processes.
- No model of a chemically reactive process is complete without it.
- It is possible to have a closed mass balance while having element balance errors.
Component Balance Equations

For component $j$:

Complete form: $\frac{dm_j}{dt} = \sum_{i=1}^{n} m_{j\text{in},i} - \sum_{i=1}^{n} m_{j\text{out},i} + f_{\text{source},j} - f_{\text{sink},j}$

Steady state form: $\sum_{i=1}^{n} m_{j\text{in},i} + f_{\text{source},j} = \sum_{i=1}^{n} m_{j\text{out},i} + f_{\text{sink},j}$

- Based on the principle of mass conservation.
- A component can refer to:
  - a chemical component,
  - a particle class with a specified set of properties,
  - any other distinguishable portion of the material in the system.
Energy Balance Equation

Generally, energy can be represented by:

\[ E_{\text{total}} = E_{\text{internal}} + E_{\text{kinetic}} + E_{\text{potential}} \]

Kinetic and potential energy can usually be neglected. We use enthalpy to account for internal energy.

- Complete form: \( \frac{d(h_{\text{in}})}{dt} = m_{\text{in}} h_{\text{in}} - m_{\text{out}} h_{\text{out}} + Q_{\text{release}} - Q_{\text{consume}} \)
- Steady state form: \( m_{\text{in}} h_{\text{in}} + Q_{\text{source}} = m_{\text{out}} h_{\text{out}} + Q_{\text{sink}} \)

- Based on the first law of thermodynamics (principle of energy conservation).
Energy Balance Equation

Process Inputs

- Inputs must be presented as accurately as possible in the mineral form, and not simply the elemental assay form. e.g. \( h_{\text{DO}} + h_{\text{CO}_2} > h_{\text{OC}_2\text{O}_4} (T = 435^\circ C) \) and \( 0.5 h_{\text{CO}_2} + h_{\text{HC}_6\text{O}_6} < h_{\text{OC}_2\text{O}_4} (T < -200^\circ C) \)
- In the case of coal, the caloric value (higher heating value, HHV), must be used to adjust enthalpy:
  \[ h_{\text{coal}} = h_{\text{elements, combusted}} + \text{HHV} \]
Other Important Equations

These equations can be used to calculate the material properties and the source and sink terms in the balance equations.
- Equations of state (physical properties as a function of T, P and composition).
- Transport processes (heat transfer, mass transfer, fluid flow).
- Chemical and phase equilibrium calculations (very powerful in pyrometallurgy).
- Chemical reaction kinetics.
Refer to Luyben (1990).
Money can be handled similar to a balance equation.

\[ \frac{dS}{dt} = \dot{m}_{\text{out}} \cdot \text{Price}_{\text{out}} + \dot{E}_{\text{out}} \cdot \text{Price}_{\text{out}} - \dot{m}_{\text{in}} \cdot \text{Price}_{\text{in}} - \dot{E}_{\text{in}} \cdot \text{Price}_{\text{in}} \]

This calculate estimates the direct process profit or loss. For a full financial picture, the process model must be embedded into a financial model of the operation. This combination is called a techno-economic model.
Literature used in this lecture:
- Luyben 1990
<table>
<thead>
<tr>
<th>Fundamental Laws</th>
<th>Mass Conservation</th>
<th>Energy Conservation</th>
<th>Others</th>
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Johan Zieniew | SAIMM Pyrometallurgical Modelling Workshop 2014 |
Pyrometallurgical Process Balances
Examples

Example 1.

Consider combustion of CH\textsubscript{4} (298K) with a sufficient amount of air (298K; composition 78% N\textsubscript{2}, 21% O\textsubscript{2}, 1% Ar) to give 2% O\textsubscript{2} in the product gas, after full combustion to CO\textsubscript{2} and H\textsubscript{2}O.

a) What is the required molar ratio of air to CH\textsubscript{4}?

b) Plot the heat released by combustion as a function of the product gas temperature, and answer the following based on the graph:
   i. What is the net calorific value of CH\textsubscript{4}?
   ii. What is the value of the adiabatic flame temperature?

Example 2.

Consider solidification of low-carbon steel which enters the continuous caster mold with a superheat of 30°C. Approximate the properties of low-carbon steel with those of pure iron. The casting speed is 1 m/min, and the section shape is a slab with thickness 250 mm. The working length of the mold is 1 m, and the average heat flux is 0.9 MW/m\textsuperscript{2}. If the temperature of the liquid steel at the mold exit is equal to the liquidus (1536°C), and the average temperature of the solidified solid shell is 1350°C, calculate the thickness of the solid shell at the mold exit. Take the density of the steel in the mold to be approximately 7000 kg/m\textsuperscript{3}.

Example 3.

Consider a blast furnace which produces 5500 tonnes of hot metal per day. The part of the furnace below the wüstite reserve zone controls the furnace energy balance. The hot blast enters the furnace at 1000°C; take the blast air to contain 79% N\textsubscript{2} and 21% O\textsubscript{2}. Calculate the expected increase in coke rate (in kg of coke per tonne of hot metal) if the heat losses (through the furnace wall) increase by 1 MW. The off-gas from the wüstite reserve zone mainly contains CO and CO\textsubscript{2} (in the ratio 2.4:1), and N\textsubscript{2}, at a temperature of 1200 K. Approximate the coke as pure carbon, which enters the wüstite reserve zone at 1200 K.

Example 4.

A process to generate "hot oxygen" was patented by Anderson\textsuperscript{1}. The principle is that part of a stream of oxygen (which is initially at ambient temperature) is used to combust a fuel gas; typically about 20% of the oxygen is consumed. The result is a hot stream of gas, which consists mainly of oxygen, together with the products of the combustion reaction. This "hot oxygen" can then be used for various process applications, such as enhancing the combustion of pulverized coal which is injected into the blast furnace.

Consider the case where oxygen, which is initially at 298 K, is used to combust methane (also at 298 K). Take the reagent and product pressures to be 1 atm. Plot the temperature of the product as a function of the proportion of the oxygen that is consumed; consider consumptions from zero to 80%, and assume that the products of the combustion reaction are only O\(_2\), CO\(_2\) and H\(_2\)O, and that no heat is transferred to the surroundings. Test whether your results agree with Figure 3 of the Anderson patent, as shown at left (and included in the Excel workbook).

Example 5.

The results of Example 4 show that the predicted product temperature agrees well with those shown in the Anderson patent for percentages oxygen consumed below \(\sim 15\%\), but diverge from the Anderson values at higher degrees of reaction. The reason for this divergence is that the assumption of full reaction (to CO\(_2\), H\(_2\)O and O\(_2\)) is not valid at high product temperatures. At high temperatures, partial dissociation of the product species, to form O, OH, N, CO and H\(_2\) (in addition to formation of CO\(_2\), H\(_2\)O and O\(_2\)) needs to be taken into account. Dissociation of the gas is endothermic, and hence the predicted gas temperature is lower if dissociation occurs.

The spreadsheet supplied to you calculates equilibrium dissociation of the gas product (using the same thermodynamic data used for the energy balances). Use this spreadsheet to plot the product gas temperature when considering dissociation, and compare with Anderson’s graph.

What are the main species in the gas phase for the case where 80% of oxygen is consumed?

Example 6.

A coal has an elemental composition (dry basis) of 74% C, 5% H, 1.5% N and 9.3% O. The ash yield is 10.2% of the dry coal mass. The ash composition is 55% SiO\(_2\), 40% Al\(_2\)O\(_3\), 5% CaO. The net calorific value of the coal is 29.9 MJ/kg.

Calculate the heat released when the coal (298K) is burnt with a 5% excess of air (298K), for product temperatures from 298K to 2400K. Assume air to contain 79% N\(_2\) and 21% O\(_2\), and assume the combustion products to be CO\(_2\), H\(_2\)O, N\(_2\), O\(_2\), SiO\(_2\), Al\(_2\)O\(_3\) and CaO.
As a first step, calculate the enthalpy of the coal at 298K, assuming the coal to consist of a mixture of an organic matrix and ash-forming minerals, with the ash-forming minerals present as SiO$_2$, Al$_2$O$_3$ and CaO.

Example 7.

Liquid steel at 1600°C contains 0.08% oxygen at tap (balance mostly Fe). Cold aluminum (298K) is added to deoxidize the steel, yielding as products steel containing 4 ppm dissolved oxygen, 0.03% dissolved aluminum, and Al$_2$O$_3$. For adiabatic conditions, what is the change in the temperature of the steel as a result of the deoxidation reaction? Heats of solution in liquid iron are as follows$^2$:

Dissolved oxygen: -117.1 kJ per mol O (relative to gaseous O$_2$)

Dissolved aluminum: -71.1 kJ per mol Al (relative to pure liquid Al)

Example 8.

Direct reduced iron (DRI) is considered as an alternative to scrap in electric furnace steelmaking. Possible increased energy consumption is one consideration. Factors affecting the change in electrical energy consumption include higher productivity with continuous feeding of DRI, and the energy required to reduce FeO (in the DRI) to Fe and for melting of the gangue in the DRI. Consider the second effects, comparing the energy requirement to melt 1 kg pure cold iron (298K), with the energy requirement to melt DRI (298K) to yield 1 kg of liquid Fe (at 1873K in both cases). In the case of DRI, cold CaO is added to give a slag composition of %CaO/%SiO$_2$=1.5, and cold oxygen is injected to oxidize any excess carbon to CO (1873K), and liquid FeO (at 1873) is available to react with the slag-forming oxides, to form a slag containing 30%FeO.

Use the KTH slag model to estimate the slag enthalpy.

How much does the answer differ if the slag model is not used, and the pure-species enthalpies of the slag components are used instead?

The composition of the DRI is as follows (mass percentages):

<table>
<thead>
<tr>
<th>Component</th>
<th>Mass Percentage</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fe</td>
<td>46.8</td>
</tr>
<tr>
<td>C</td>
<td>45</td>
</tr>
<tr>
<td>FeO</td>
<td>6</td>
</tr>
<tr>
<td>SiO$_2$</td>
<td>1.2</td>
</tr>
<tr>
<td>CaO</td>
<td>0.8</td>
</tr>
<tr>
<td>Al$_2$O$_3$</td>
<td>0.2</td>
</tr>
</tbody>
</table>

Example 9.

In electric furnace steelmaking, the presence of carbon in the melt helps to remove nitrogen by “carbon boil”; the result is that the average nitrogen content at tap is lower.

if the melt-in carbon content is higher; see the figure below. The following relationship approximately fits the plant data:

\[
[\text{ppm } N_{\text{tap}}] = 45 + 36 \exp (-6[\%C]_{\text{melt-in}})
\]

One possible way for such a relationship to arise is if the kinetics of nitrogen removal is limited by mass transfer, specifically the availability of CO bubbles. For such a case of gas flow rate limitation, the CO bubbles would be saturated with N\(_2\) upon leaving the metal bath; the relationship between the mole fraction of nitrogen in the bubbles (at any stage of the steelmaking process after melt-in) and the mass percentage of nitrogen remaining in the steel at that stage is then simply given by Sieverts’ law:

\[
[\text{ppm } N] = K(p_{N_2})^{0.5}, \text{ where } K=450 \text{ at } 1600^\circ\text{C}.
\]

For this mass-transfer limited case, it can be shown that the relationship between the mass percentage of nitrogen remaining in the steel after removal of a certain percentage of carbon is as follows:

\[
\frac{1}{\text{ppm } N} - \frac{1}{\text{ppm } N_0} = \left( \frac{n_{\text{gas}}}{W_{\text{steel}}} \right) \left( \frac{M_{N_2}}{K^2 p_{\text{tot}}} \right)
\]

where \(n_{\text{gas}}\) is the total amount of CO evolved (in mol), \(W_{\text{steel}}\) is the steel mass in tons, \(M_{N_2}=28\) g/mol is the molar mass of \(N_2\), \(K=450\) as stated, and \(p_{\text{tot}}\) is the total pressure in atmospheres.

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Test whether, for this electric furnace plant, the removal of nitrogen is limited by the rate of supply of CO, such that the CO bubbles are saturated with nitrogen upon leaving the bath.
Mass and Energy

**Why mass and energy balances?**
- All processes need to balance mass and energy requirements
- Heat transfer is limiting in many processes

Endothermic, e.g. Carbon-based reduction of metal oxides

Exothermic, e.g. solidification
Mass and energy balances test process feasibility

(VirtualFunHouse.com, after MC Escher)
Principles of mass & energy balances

- “Black-box” approach
  - Mass and heat transfer across system boundary tallied
- Steady-state or dynamic
- No detail of individual chemical reactions required, other than:
  - stoichiometry (each component must balance)
  - extent of chemical reactions, based on:
    - reasonable assumptions
    - and/or reaction equilibria
    - and (when needed) reaction kinetics
Example: Predicted effect of metallic feed only fuel rate and productivity of a blast furnace

Fe° input beneficial; metallization of DRI has little effect

(Pistorius, TMS2012)
Information *not* directly supplied by mass & energy balances

- **Reaction equilibria**
  - addressed with multicomponent equilibrium calculations (e.g. FactSage)

- **Equipment sizing**
  - addressed with mass and heat transfer & reaction kinetics calculations (e.g. CFD)
Energy balance principles

- Normally based on enthalpy, for pyrometallurgical processing

System Properties:
- volume, mass, temperature, 
- $U'$, $S'$, $G'$, $H'$...

Heat transfer $\Delta q$

Mass transfer $\Delta m$

All the system properties can change in response to heat & mass transfer
For system that remains at constant pressure:

\[ \Delta q = \Delta H' \]

Net heat transferred into system (in joule) \quad Change in enthalpy of system (in joule)

Enthalpy balances commonly used to calculate net heat transfer; only valid if the system pressure remains constant.
Calculating enthalpy changes:

\[ \Delta H' = \left( \sum n_i H_i \right)_{\text{after}} - \left( \sum n_i H_i \right)_{\text{before}} \]

- Molar amount of each species in its appropriate chemical state
- Molar enthalpy of each species (in J/mol);
  \[ H_i = H_i^o + \Delta \bar{H}_{ex,i} \]

Enthalpy of pure species

Heat of solution
The energy balance starts with a mass balance

- To calculate all the $n_i$ terms
- Principle: stoichiometry
- Mass balance based on:
  - Concentrations of components (relevant compounds and elements) in reactants and products
  - Molar balances for all components
- Important convention for compositions:
  - Condensed phases (solids & liquids): mass percentages;
  - Gases: molar percentages
Example 1
Consider combustion of CH$_4$ (298K) with a sufficient amount of air (298K; composition 78% N$_2$, 21% O$_2$, 1% Ar) to give 2% O$_2$ in the product gas, after full combustion to CO$_2$ and H$_2$O(g).

a) What is the required molar ratio of air to CH$_4$?

b) Plot the heat released by combustion as a function of the product gas temperature, and answer the following based on the graph:
   i. What is the net calorific value of CH$_4$?
   ii. What is the value of the adiabatic flame temperature?
Mass balance procedure followed here

- Choose basis (e.g. 1 mol input, or 1 tonne product)
- Tabulate identity, molar amount, and mass of each species (inputs & products)
- Total mass of inputs; compare with mass of outputs
  - Difference: accumulated mass
    - zero for steady state
  - For “integrating” system:
    initial mass + mass of inputs = final mass
- Total masses must balance exactly
- Each component must also balance exactly
### Example 1

Inputs: CH\(_4\), air (78% N\(_2\), 21% O\(_2\), 1% Ar)

Products: CO\(_2\), H\(_2\)O, N\(_2\), O\(_2\), Ar

Choose basis: 1 mol CH\(_4\)

How much air required to give 2% O\(_2\) in product gas?

Designate the molar amount of air as \(x\).

Molar amounts of components in product:
- 1 mol CO\(_2\); (to balance carbon in 1 mol CH\(_4\))
- 2 mol H\(_2\)O; (to balance hydrogen in 1 mol CH\(_4\))
- 0.21\(x\)-\((1+0.5\times2)\) mol O\(_2\)
  (input in air minus that in CO\(_2\) and H\(_2\)O)
- 0.78\(x\) mol N\(_2\); 0.01\(x\) mol Ar
Example 1
Total moles of product gas:
\[ 1 + 2 + 0.21x - 2 + 0.78x + 0.01x = 1 + x \]
Mole fraction of oxygen in product gas
\[ \frac{(0.21x - 2)}{(1 + x)} = 0.02 \]
Solve for \( x = 10.63 \)
Example 1
a) What is the required molar ratio of air to CH₄?
b) Plot the heat released by combustion as a function of the product gas temperature

Draw up the mass balance in tabular form
<table>
<thead>
<tr>
<th>Species</th>
<th>M (kg)</th>
<th>m (mol)</th>
<th>T (K)</th>
<th>Assumed basis</th>
<th>See Excel table</th>
</tr>
</thead>
<tbody>
<tr>
<td>CH₄</td>
<td>0.016</td>
<td>0.016</td>
<td>298</td>
<td>1.000</td>
<td></td>
</tr>
<tr>
<td>N₂</td>
<td>0.028</td>
<td>8.293</td>
<td>298</td>
<td></td>
<td></td>
</tr>
<tr>
<td>O₂</td>
<td>0.032</td>
<td>2.233</td>
<td>298</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Ar</td>
<td>0.004</td>
<td>0.106</td>
<td>298</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Total</td>
<td>0.324</td>
<td>0.324</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Inputs:**

- CO₂
  - 2500 K
  - 1.000 mol
  - 0.044 kg/mol
  - 0.044 kg
- H₂O
  - 2500 K
  - 2.000 mol
  - 0.018 kg/mol
  - 0.036 kg
- N₂
  - 2500 K
  - 8.293 mol
  - 0.028 kg/mol
  - 0.232 kg
- O₂
  - 2500 K
  - 0.233 mol
  - 0.032 kg/mol
  - 0.007 kg
- Ar
  - 2500 K
  - 0.106 mol
  - 0.04 kg/mol
  - 0.004 kg

**Products:**

- CO₂
  - 2500 K
  - 1.000 mol
  - 0.044 kg/mol
  - 0.044 kg
- H₂O
  - 2500 K
  - 2.000 mol
  - 0.018 kg/mol
  - 0.036 kg
- N₂
  - 2500 K
  - 8.293 mol
  - 0.028 kg/mol
  - 0.232 kg
- O₂
  - 2500 K
  - 0.233 mol
  - 0.032 kg/mol
  - 0.007 kg
- Ar
  - 2500 K
  - 0.106 mol
  - 0.04 kg/mol
  - 0.004 kg

**Total:**

- 0.324 kg/mol
- 0.324 kg

Must agree exactly
Example 1
a) What is the required molar ratio of air to CH₄?

b) Plot the heat released by combustion as a function of the product gas temperature

Draw up the mass balance in tabular form.

Next: find and insert enthalpies for all the species at the appropriate temperatures.

Approach used here:
thermodynamic data from NIST Chemistry WebBook
(open-source version of JANAF tables);
http://webbook.nist.gov/chemistry/
### Constants from NIST

<table>
<thead>
<tr>
<th>T-max</th>
<th>1200</th>
<th>6000</th>
</tr>
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<tbody>
<tr>
<td>A</td>
<td>-0.393079</td>
<td>85.81237</td>
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<tr>
<td>B</td>
<td>108.6771</td>
<td>15.26467</td>
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<td>C</td>
<td>42.52157</td>
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<tr>
<td>D</td>
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<td>E</td>
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<tr>
<td>F</td>
<td>78.84376</td>
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</tr>
<tr>
<td>G</td>
<td>158.2163</td>
<td>224.4143</td>
</tr>
</tbody>
</table>

**T-max:** Maximum temperature (in kelvin) to which constants are valid

Cells which calculate $H^\circ$, $S^\circ$ & $G^\circ$

**Cp:** heat capacity (J/mol*K)

**$H^\circ$:** standard enthalpy (kJ/mol)

**$S^\circ$:** standard entropy (J/mol*K)

**$T$:** temperature (K) / 1000

<table>
<thead>
<tr>
<th>T (K)</th>
<th>Range</th>
<th>$H^\circ$ (kJ/mol)</th>
<th>$S^\circ$ (kJ mol K$^{-1}$)</th>
<th>$G^\circ$ (kJ/mol)</th>
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</thead>
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<td>500</td>
<td>1</td>
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</table>
Completed calculation

<table>
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<tr>
<th>Species</th>
<th>T (K)</th>
<th>n (mol)</th>
<th>M (kg/mol)</th>
<th>m (kg)</th>
<th>H (J/mol)</th>
<th>nH (J)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Inputs:</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>CH(_4)</td>
<td>298</td>
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<td>0.016</td>
<td>0.016</td>
<td>-74877.2</td>
<td>-74877</td>
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<td>8.293</td>
<td>0.028</td>
<td>0.232</td>
<td>-4</td>
<td>-36</td>
</tr>
<tr>
<td>O(_2)</td>
<td>298</td>
<td>2.233</td>
<td>0.032</td>
<td>0.071</td>
<td>-5</td>
<td>-10</td>
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<tr>
<td>Ar</td>
<td>298</td>
<td>0.106</td>
<td>0.04</td>
<td>0.004</td>
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<td>0</td>
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<tr>
<td>Total</td>
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<td></td>
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<td>-74924</td>
</tr>
<tr>
<td>Products:</td>
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<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>CO(_2)</td>
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<td>1.000</td>
<td>0.044</td>
<td>0.044</td>
<td>-360123</td>
<td>-360123</td>
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<tr>
<td>H(_2)O</td>
<td>1000</td>
<td>2.000</td>
<td>0.012</td>
<td>0.036</td>
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<td>-431648</td>
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<tr>
<td>N(_2)</td>
<td>1000</td>
<td>8.293</td>
<td>0.028</td>
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<tr>
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<td>0.032</td>
<td>0.007</td>
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<td>0.04</td>
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<td></td>
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<td></td>
<td>0.324</td>
<td>-606956</td>
</tr>
</tbody>
</table>

\[\Delta q = \Delta H' = -532032\]

Heat released = \(-\Delta q = 532 \text{ kJ (for 1 mol CH}_4\text{)}\)
Heat released = 33.3 MJ (for 1 kg CH\(_4\))
Skills to practise with this example
1. Tabular form of mass balance
2. Use Excel enthalpy correlations
   - transfer temperature with link, **not** by entering value;
   - transfer enthalpy with link, **not** by entering value
Example 2.
Consider solidification of low-carbon steel (≈pure iron) which enters the continuous caster mold with a superheat of 30°C.
The casting speed is 1 m/min, and the section shape is a slab with thickness 250 mm.
The working length of the mold is 1 m, and the average heat flux is 0.9 MW/m².
The temperature of the liquid steel at the mold exit is 1536°C and the average temperature of the solidified solid shell is 1350°C.
Calculate the thickness of the solid shell at the mold exit.
Mold region = system considered

1 MW

solid shell

Inflow of liquid steel

0.125 m

Casting direction

Outflow of solid shell and remaining liquid steel
From casting speed

<table>
<thead>
<tr>
<th>Consider</th>
<th>1 s of casting, half the slab thickness, and 1 m of slab width.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Estimated solid shell thickness:</td>
<td>0.0200 m</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Species</th>
<th>T (K)</th>
<th>n (mol)</th>
<th>M (kg/mol)</th>
<th>n (kg)</th>
<th>H (J/mol)</th>
<th>nH (J)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Inputs:</td>
<td>Fe-liqu</td>
<td>1839</td>
<td>261.1161</td>
<td>0.05585</td>
<td>14.58</td>
<td>73833</td>
</tr>
<tr>
<td>Total</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Products:</td>
<td>Fe-liqu</td>
<td>1809</td>
<td>219.3375</td>
<td>0.05585</td>
<td>12.25</td>
<td>72452</td>
</tr>
<tr>
<td></td>
<td>Fe-shell</td>
<td>1623</td>
<td>41.77837</td>
<td>0.05585</td>
<td>2.33</td>
<td>50210</td>
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<tr>
<td>Total</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Heat transferred into system: -1290195

From assumed shell thickness

Calculated heat extracted = 1.29 MJ
Should be 0.9 MJ ⇒ assumed shell too thick
Possible approaches to finding the correct thickness:

- Trial and error
- “Goal seek”
- Recommended method: iterative calculation
- Principle: let $x$ be the target variable (e.g. shell thickness)

$$x_{\text{new}} = x_{\text{old}} - \omega \frac{\text{Error}}{\text{sensitivity}}$$

- New estimate of shell thickness
- Error in target function, e.g. $1.29 \text{ MJ} - 0.9 \text{ MJ}$
- Change in error with change in $x$
For the current example:
At x=0.02 m, error = 1.29-0.9 = 0.39 MJ
Try another thickness:
at x=0.01 m, error = 0.83-0.9 = -0.07 MJ
⇒ Sensitivity = (-0.07 – 0.39) / (0.01-0.02) = 46 MJ/m
⇒ Starting from x=0.01 m, the new estimate is:
   \[ x_{\text{new}} = 0.01 - \omega(-0.07/46) = 0.01 + 0.0015\omega \]

What is \( \omega \)?
- Relaxation factor; avoids unstable oscillations
  if sensitivity is poorly known or varies with x
- Typically use \( \omega = 0.1 \)
### Pyrometallurgical Modelling Principles and Practices

**Formula to enter in this cell:**

=IFERROR(D26,0.03)

<table>
<thead>
<tr>
<th>Species</th>
<th>T (K)</th>
<th>n (mol)</th>
<th>M (kg/mol)</th>
<th>m (kg)</th>
<th>H (J/mol)</th>
<th>nH (J)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fe-liquid</td>
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<td>261.1161</td>
<td>0.05585</td>
<td>14.58</td>
<td>73833</td>
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<tr>
<td>Total</td>
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<td></td>
</tr>
<tr>
<td>Fe-solid</td>
<td>1809</td>
<td>240.2268</td>
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<td>Total</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Heat transferred into system:** 825362 J

- Heat transferred in 1 second: 0.825 MJ (out of steel)
- Error in estimate: -0.075 MJ
- Estimated sensitivity: 46 MJ/m
- Relaxation factor for iteration: 0.1 (~0.1)
- New estimate of shell thickness: 0.010162 m

**Cell D26**
What does the statement IFERROR(D26,0.03) do?

- Current value of cell D26 inserted into the current cell, unless a calculation error results (e.g. diverging calculation)
- If an error results, the default value (0.03 in this case) is inserted instead

Excel will probably alert you to a circular reference. Go to File – Options – Formula, and ensure that “Enable iterative calculation” is checked.
Performing an energy balance for just part of a larger system:
Example 3.
A blast furnace produces 5500 tonnes of hot metal per day.
The part of the furnace below the würstite reserve zone controls the furnace energy balance. The hot blast (79% N₂ - 21% O₂) enters the furnace at 1000°C. Calculate the expected increase in coke rate (in kg of coke per tonne of hot metal) if the heat losses (through the furnace wall) increase by 1 MW.
The off-gas from the würstite reserve zone mainly contains CO and CO₂ (in the ratio 2.4:1), and N₂, at a temperature of 1200 K. Approximate the coke as pure carbon, which enters the würstite reserve zone at 1200 K.
Full blast furnace mass and energy balance; based on known conditions in the chemical reserve zone (T≈1200K; Fe-FeO-CO-CO₂-H₂-H₂O equilibrium)

Coke rate and blast air requirement calculated:

Fe₀.₉₅O, Fe°, C, gangue, fluxes - 1200 K

CO, CO₂, H₂, H₂O, N₂; 1200 K known X₃/CO₂ and X₃/H₂O

O₂, N₂, H₂O, coal - Tblast

SiO₂-Al₂O₃-CaO-MgO-MnO slag

Fe-C-Si-Mn hot metal - Ttap

The full model predicts an increase in C rate of ~0.95kg/THM for 1MW higher heat loss (5.5kTHM/day)
Rephrasing the specific question:
At what rate must pure C (1200K) be burnt with air (79% N₂ - 21% O₂; 1273K) to yield CO & CO₂ (2.4:1) and N₂ as products (1200K) to give a heat transfer rate of 1 MW.
Recommended approach: (1kg C as basis)
Use carbon mass balance to find molar amounts of CO & CO$_2$ in product;
find O$_2$-input from oxygen reporting to product (as CO and CO$_2$); find N$_2$ from O$_2$-input.
Complete energy balance

<table>
<thead>
<tr>
<th>Species</th>
<th>T (K)</th>
<th>n (mol)</th>
<th>M (kg/mol)</th>
<th>m (kg)</th>
<th>H (J/mol)</th>
<th>nH (J)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Inputs:</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>1200</td>
<td>0.012</td>
<td>1</td>
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<tr>
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<td>1273</td>
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</tr>
<tr>
<td>O$_2$</td>
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<td>Total</td>
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<td></td>
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</tr>
<tr>
<td>Products:</td>
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<td>CO</td>
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<tr>
<td>N$_2$</td>
<td>1200</td>
<td>0.028</td>
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<tr>
<td>Total</td>
<td></td>
<td></td>
<td></td>
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<td></td>
<td></td>
</tr>
</tbody>
</table>

Recommended approach: (1kg C as basis)
Use carbon mass balance to find molar amounts of CO & CO$_2$ in product;
find O$_2$-input from oxygen reporting to product (as CO and CO$_2$); find N$_2$ from O$_2$-input.
Complete energy balance
Calculating product temperature
All the previous examples: temperatures of inputs & products known
Also often required: calculate the product temperature, for a given amount of heat transferred
Next example: product temperature calculated for adiabatic conditions.
Adiabatic ⇒ no heat transfer, so Δq = 0;
\[ (\sum n_i H_i)_{\text{after}} = (\sum n_i H_i)_{\text{before}} \]
Example 4: “Hot oxygen” burner

(Oxygen, Fuel, Hot oxygen-rich gas)

(Anderson, US Pat 5,266,024 [1993])
Example 4.
Part of a stream of oxygen (298K) is used to combust methane (298K); the result is a hot stream of gas, which consists of unreacted oxygen, together with the products of the combustion reaction. Plot the temperature of the product as a function of the proportion of the oxygen that is consumed; consider consumptions from zero to 80%; assume that the products are only O₂, CO₂ and H₂O, and that no heat is transferred to the surroundings.
Methane input: \( \text{CH}_4 + 2\text{O}_2 = \text{CO}_2 + 2\text{H}_2\text{O} \Rightarrow 1 \text{ mol O}_2 \) reacts with 0.5 mol CH\(_4\)

Calculate from fraction O\(_2\) reacted

Set as input value
Example 4.
For iterative calculation of product temperature:
Link temperature in enthalpy worksheets to relevant

  cell in energy balance worksheet;

  link enthalpy in energy balance worksheet with

  relevant cells in enthalpy worksheets
Example 4: Reported flame temperature

(per Anderson, US Pat 5,266,024 [1993])
Calculated temperatures deviate from those reported by Anderson at high fractions $O_2$ reacted.
Reason for deviation:

- Product does not contain only O\textsubscript{2}, CO\textsubscript{2} and H\textsubscript{2}O
- Also present: O, CO, H\textsubscript{2}, H, OH
  - dissociation occurs
- Dissociation is endothermic
  \( \Rightarrow \) lower product temperature

Example 5.
Test the effects of dissociation on product gas composition and adiabatic flame temperature. Available spreadsheet takes into account multicomponent equilibria.
Example 6: Coal

- Coal is complex mixture of organic compounds and minerals

Proposed structure of bituminous coal (van Heek, 2000)
Ground coal: microscopic appearance
(back-scattered electron image)
# Minerals in coal

<table>
<thead>
<tr>
<th>Common minerals</th>
<th>Formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>Kaolinite</td>
<td>Al₂Si₂O₅(OH)₄</td>
</tr>
<tr>
<td>Quartz</td>
<td>SiO₂</td>
</tr>
<tr>
<td>Pyrite</td>
<td>FeS₂</td>
</tr>
<tr>
<td>Illite</td>
<td>(K₁₋₁.₅)Al₄<a href="OH">Si₇₋₆.₅Al₁₋₁.₅O₂₀</a>₄</td>
</tr>
<tr>
<td>Apatite</td>
<td>Ca₅(PO₄)₃(Cl,OH)</td>
</tr>
</tbody>
</table>
Reasonable approach to handling this complexity:

Mass balance:

- Elemental analysis (C, H, N, O, S) of organic part ("Ultimate analysis")
- Use ash analysis to approximate mineral composition
  Ash – residue after coal is combusted completely; composition of ash is not identical with that of minerals in coal

Energy balance:

- Use calorific value to calculate coal enthalpy at 298K.
**Calorific values:**
- Heat released when fuel is combusted completely; temperature of products equal to that of reactants
- Temperature strictly speaking 273K; using 298K gives essentially the same result
- Net calorific value: \( H_2O \) in product as vapor
- Gross calorific value: \( H_2O \) in product as liquid
**Example 6: Coal**

A coal has an elemental composition (dry basis) of 74% C, 5% H, 1.5% N and 9.3% O.
The ash yield is 10.2% of the dry coal mass.
The ash composition is 55% SiO$_2$, 40% Al$_2$O$_3$, 5% CaO.
The net calorific value of the coal is 29.9 MJ/kg.

Calculate the enthalpy of the coal at 298K, assuming the coal to consist of a mixture of an organic matrix and ash-forming minerals, with the ash-forming minerals present as SiO$_2$, Al$_2$O$_3$ and CaO.
To be completed, based on coal composition
Values from NIST correlations
Calorific value
Calculate once other values have been entered

<table>
<thead>
<tr>
<th>Species</th>
<th>T (K)</th>
<th>n (mol)</th>
<th>M (kg/mol)</th>
<th>m (kg)</th>
<th>H (J/mol)</th>
<th>n (J)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Inputs:</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Coal</td>
<td>298</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>O₂</td>
<td>298</td>
<td>1</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Total</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Products:</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>CO₂</td>
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<td></td>
<td></td>
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<td></td>
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<tr>
<td>H₂O</td>
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<td></td>
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<td></td>
<td></td>
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<tr>
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</tr>
<tr>
<td>SO₂</td>
<td>298</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Al₂O₃</td>
<td>298</td>
<td></td>
<td></td>
<td></td>
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<td></td>
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<tr>
<td>CaO</td>
<td>298</td>
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<td></td>
<td></td>
</tr>
<tr>
<td>Total</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Heat released</td>
<td>29900000 J</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

To be completed, based on coal composition
Values from NIST correlations
Calorific value
Example 6: Coal

Next: use this known coal enthalpy to calculate the heat released when the coal (298K) is burnt with a 5% excess of air (298K), for product temperatures from 298K to 2400K.

Assume air to contain 79% N₂ and 21% O₂, and assume the combustion products to be CO₂, H₂O, N₂, O₂, SiO₂, Al₂O₃ and CaO.

- Similar to Example 1
Example 7: Heats of solution

Most input and product streams are not pure elements or pure compounds; most are non-ideal solutions.

- Heat of solution must generally be taken into account, for condensed phases (solids & liquids).
- Heat of solution simply adds to pure-species enthalpy:

\[ H_i = H_i^0 + \Delta H_{ex,i} \]

**Diagram:**
- Enthalpy of pure species
- Heat of solution
Example 7: Heats of solution

Heat of solution primarily depends on:
- species
- solvent (e.g. different for steel and hot metal)

Weaker dependence on concentration & temperature

Find heats of solution from:
- literature correlations
- thermodynamic model for the solution phase
Example 7
Liquid steel at 1600°C contains 0.08% oxygen at tap (balance mostly Fe).
Cold aluminum (298K) is added to deoxidize the steel, yielding as products steel containing 4 ppm dissolved oxygen, 0.03% dissolved aluminum, and Al₂O₃.
For adiabatic conditions, what is the change in the temperature of the steel as a result of the deoxidation reaction?

Heats of solution in liquid iron are as follows:
Dissolved oxygen:
-117.1 kJ per mol O (relative to gaseous O₂)
Dissolved aluminum:
-71.1 kJ per mol Al (relative to pure liquid Al)
$H_O = 0.5H_{O_2} + \Delta H_s$

<table>
<thead>
<tr>
<th>Species</th>
<th>T (K)</th>
<th>n (mol)</th>
<th>M (kg/mol)</th>
<th>m (kg)</th>
<th>H (J/mol)</th>
<th>nH (J)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Inputs:</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
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<td>0.05585</td>
<td>0.99992</td>
<td>-92200</td>
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</tr>
<tr>
<td>O</td>
<td>1873</td>
<td>0.05</td>
<td>0.016</td>
<td>0.00082</td>
<td>-4494.96</td>
<td>-4494.96</td>
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<tr>
<td>Al</td>
<td>208</td>
<td>0.044272</td>
<td>0.027</td>
<td>0.00120</td>
<td>-0.176052</td>
<td>-0.176052</td>
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<td></td>
<td>1.00120</td>
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</tr>
<tr>
<td>Fe</td>
<td>1920</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>O</td>
<td>1920</td>
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<td></td>
<td></td>
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<tr>
<td>Al</td>
<td>1920</td>
<td></td>
<td></td>
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<tr>
<td>Al_{2}O_{3}</td>
<td>1920</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
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<td>Total</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>1.00120</td>
<td>1362980</td>
</tr>
</tbody>
</table>

Estimated temperature after deoxidation: 1920.0 K
Heat transferred to system: 18558.1 J
Estimated sensitivity: 826 J/K
Relaxation factor for iteration: 0.1 [-u]
New estimate of temperature: 1917.8 K
Example 8: Slag enthalpy

Slags are concentrated, non-ideal solutions
- Heat of solution significant

Heat of solution can strongly affect energy balance of processes with high slag volumes, e.g. platinum smelting, ferronickel & other ferroalloys

In general:
slag enthalpy evaluated using solution model

Approach used here: KTH slag model
### Example 8: Slag enthalpy

Compare energy required to melt direct-reduced iron (DRI), with energy required to melt pure iron.

DRI contains carbon (as Fe₃C), unreduced FeO, and gangue oxides. React to form Fe and CO (endothermic); excess C oxidized by O₂ (exothermic).

React with CaO (exothermic) and melt (endothermic) to form slag.

Slag composition: (%CaO)/(%SiO₂)=1.5; 30%FeO
Calculate DRI mass from total Fe percentage in DRI, and 1 kg of Fe product

Do not calculate enthalpy of each slag oxide

Instead: see next slide
Slag enthalpy: KTH model*

Interaction between oxides in molten slag considered

Enter slag composition (mass %) and temperature (%SiO$_2$) calculated by difference; slag enthalpy reported per mol and per kg (more useful)

---

Example 8: Slag enthalpy

How strong is the effect of heat of mixing in the slag?

Test by repeating calculation, using enthalpies of individual liquid oxides, instead of overall slag enthalpy.
Example 9: Kinetics

Rates of many processes limited by mass & energy balance.
Examples:

- Continuous casting
  - solidification rate determined by heat transfer
- Ferroalloy production
  - metal production rate $\propto$ power input
- Blast furnace ironmaking
  - hot metal production rate $\propto$ blowing rate
- Oxygen steelmaking (only for [%C]>0.3%)
  - decarburization rate $\propto$ oxygen blowing rate
Removal of dissolved nitrogen by carbon boil

CO bubbles

[N]

liquid steel containing dissolved C and N

Nitrogen flushed out by CO:

\[
[N]_{\text{steel}} = 0.5(N_2)_{\text{g}} \quad \text{equilibrium [ppm N]} = 450(p_{N_2})^{0.5}
\]
Example 9: Is N removal limited by CO availability?
Possibility tested:
Each CO bubble leaves steel saturated with N₂
Expected relationship:
\[
\frac{1}{\text{ppm}N} - \frac{1}{\text{ppm}N_0} = \frac{n_{\text{gas}}}{W_{\text{steel}}} \left( \frac{M_{\text{N}_2}}{K^2P_{\text{tot}}} \right)
\]
\([N]\) after carbon boil
\([N]\) before carbon boil
(take as 81 ppm)
steel mass (in tonnes)
Moles of CO evolved
molar mass of \(N_2=28\text{g/mol}\)
1 atm
\(K=450\)
Example 9: Is N removal limited by CO availability?

Test whether the predicted relationship agrees with the plant data

Removal of dissolved nitrogen by carbon boil: EAF plant data*

Mass and Energy - Practical Work
Techno Economic Modelling
BF Plus – Practical Work
Cost Example

Example 10

In this example, we estimate the overall cost of converting an existing blast furnace to the "BF plus" concept (see diagram below)\(^5\). In this concept, the blast furnace top gas is intentionally engineered to have a high calorific value. This would yield a top gas which would be suitable for power generation using a combined-cycle power plant (that uses both a gas turbine, “GT” in the diagram below, and a heat-recovery steam generator and steam turbine – “HRSG” and “ST” in the diagram).

To generate the high volume of calorific topgas, the pulverized coal injection rate would be increased dramatically, the blast temperature would be decreased, and oxygen enrichment of the blast air wold be increased.

The capital expenditure comprises the air separation unit (to produce the additional oxygen), expanded coal handling and pulverizing, and combined-cycled power plant. The cost of capital is to be calculated by assuming a project life of 15 years and a discount rate of 10%. Cost of lost production is not included.

Estimate the difference in cost between a base-case conventional blast furnace, and the same furnace if it were converted to the “BF-plus” concept. The accompanying spreadsheet will guide you through the calculation procedure. The spreadsheet includes values calculated from a furnace mass and energy balance, including coke rate, blast rate, and topgas rate and calorific value.

Express the final difference in cost in US$ per tonne of hot metal (THM).
Assumptions

Price for electricity (generation only): 6c per kWh\(^6\)

Energy efficiency of blast furnace stoves: 60% (relative to net heating value of fuel gas)\(^7\)

Coke price $220 per short ton\(^8\)

Coal price $60 per short ton\(^9\)

Efficiency of electricity generation: 55% (relative to the net heating value of the fuel gas)\(^11\)

**Plant capital costs** are given for a specific reference year, and are converted to 2012 costs by the conversion

\[ C_i = C_{i,\text{ref}} \times \left( \frac{\text{PCI}}{\text{PCI}_{\text{ref}}} \right) \]

where \( C_i \) is the cost of unit \( i \), \( C_{i,\text{ref}} \) the cost of the unit in the reference year, PCI is the process cost index for the current year, and PCI\(_{\text{ref}}\) the cost in the reference year.

Plant cost indices are tabulated below (from *Chemical Engineering Magazine*, www.che.com)

<table>
<thead>
<tr>
<th>Year</th>
<th>Plant cost index</th>
<th>Year</th>
<th>Plant cost index</th>
<th>Year</th>
<th>Plant cost index</th>
</tr>
</thead>
<tbody>
<tr>
<td>1977</td>
<td>204.1</td>
<td>1990</td>
<td>357.6</td>
<td>2003</td>
<td>402.0</td>
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<tr>
<td>1978</td>
<td>218.8</td>
<td>1991</td>
<td>361.3</td>
<td>2004</td>
<td>444.2</td>
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<tr>
<td>1979</td>
<td>238.7</td>
<td>1992</td>
<td>358.2</td>
<td>2005</td>
<td>468.2</td>
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<tr>
<td>1980</td>
<td>261.1</td>
<td>1993</td>
<td>359.2</td>
<td>2006</td>
<td>499.6</td>
</tr>
</tbody>
</table>

---


\(^{8}\) www.eia.gov/coal/production/quarterly/pdf/t17p01p1.pdf

\(^{9}\) www.eia.gov/coal/annual/pdf/table31.pdf
Capital cost: pulverized-coal plant

Use figures from the US National Energy Technology Laboratory (NETL) to estimate the capital cost of additional pulverized coal\textsuperscript{10}, assuming a capacity factor of 1. According to that report, a pulverized-coal plant (including conveying the pulverized coal) costs around US$46 million (2007 dollars) for a plant with a capacity of 5000 tonnes of coal per day.


<table>
<thead>
<tr>
<th>Year</th>
<th>Cost 1</th>
<th>Cost 2</th>
<th>Cost 3</th>
<th>Cost 4</th>
<th>Cost 5</th>
</tr>
</thead>
<tbody>
<tr>
<td>1981</td>
<td>297.0</td>
<td>199.4</td>
<td>368.1</td>
<td>2007</td>
<td>525.4</td>
</tr>
<tr>
<td>1982</td>
<td>314.0</td>
<td>199.5</td>
<td>381.1</td>
<td>2008</td>
<td>575.4</td>
</tr>
<tr>
<td>1983</td>
<td>316.9</td>
<td>199.6</td>
<td>381.7</td>
<td>2009</td>
<td>521.9</td>
</tr>
<tr>
<td>1984</td>
<td>322.7</td>
<td>199.7</td>
<td>386.5</td>
<td>2010</td>
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<tr>
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<td>199.8</td>
<td>389.5</td>
<td>2011</td>
<td>585.7</td>
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<td>1986</td>
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<td>199.9</td>
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<td>1988</td>
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<td>394.3</td>
<td>Mar. 2104</td>
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<tr>
<td>1989</td>
<td>355.4</td>
<td>200.2</td>
<td>395.6</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Capital cost: power plant

Use NETL figures for a natural gas combined-cycled plant to estimate the capital cost (total as-spent cost) and operating cost (fixed and variable) of the combined-cycle power plant, assuming a capacity factor of 1.

According to the NETL, the total plant cost of a combined-cycle plant with a net output power of 555 MW in 2007 dollars is US$325 million.

Capital cost of air separation unit (reference costs in thousands of year 1989 dollars).
(take \( N_t = N_o \) and \( T_a = 60^\circ F \). Note that 1 lbmole = 0.454 kmol; assumed oxygen purity to be 97.5%)

\[
C_{ASU,\text{ref}} = \frac{14.35 \times N_t \times T_a^{0.067}}{(1 - \phi)^{0.073}} \left( \frac{M_{ax}}{N_o} \right)^{0.852}
\]

where,

- \( T_a \) = Ambient air temperature (\(^\circ F\))
- \( N_t \) = Total number of production trains
- \( N_o \) = Number of operating production trains
- \( M_{ax} \) = Molar flow rate of output oxygen (not oxygen product) (lbmole/hr)
- \( \phi \) = Purity of oxygen product
- \( 20^\circ F \leq T_a \leq 95^\circ F \)
- \( 625 \leq \left( \frac{M_{ax}}{N_o} \right) \leq 11.350 \) lbmole/hr
- \( 0.95 \leq \phi \leq 0.995 \)

Total plant cost of air separation unit

The total plant cost is more than the cost of the individual pieces of equipment (the "process facilities capital", PFC, calculated using the correlation given above). The total plant cost includes engineering office expenses, general facilities, project and process contingencies, and royalty fees. These amount to another 37.5% of the PFC.

---


Power requirement: air separation unit (oxygen plant)

MACP = 0.0049*φ + 0.4238, for φ ≤ 97.5%

where,
- MACP = kWh/100 ft³ O₂ product
- φ = O₂ product purity (mole%)

Take the oxygen purity to be 97.5%
(reference conditions for volume in standard cubic feet: 60°F, 1 atm pressure)

Power requirement: Compression of top gas.

Compression of the fuel gas (blast furnace top gas) before it is fed to the gas turbine typically consumes about 162 kW of power for every 1000 scf per minute of blast furnace gas being compressed.

Operating costs: air separation unit (oxygen plant)

<table>
<thead>
<tr>
<th>O&amp;M Cost Elements</th>
<th>Typical Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fixed O&amp;M Costs</td>
<td></td>
</tr>
<tr>
<td>Total Maintenance Cost</td>
<td>4% TPC</td>
</tr>
<tr>
<td>Maintenance Cost Allocated to Labor (f_{maintlab})</td>
<td>40% of total maint. Cost</td>
</tr>
<tr>
<td>Admin. &amp; Support Labor Cost (f_{admin})</td>
<td>30% of total labor cost</td>
</tr>
<tr>
<td>Operating Labor (N_{labor})</td>
<td>2 jobs/shift</td>
</tr>
</tbody>
</table>

Fixed cost of labor:

\[ FOM_{labor} = \text{labour} \times N_{labor} \times 40(\text{hrs/week}) \times 52(\text{weeks/yr}) \]

\[ \text{labour} = \text{the hourly wages to the labor ($/hr) = $24.82/hr} \]

\[ \text{Admin & support labor cost} = f_{admin} \times [FOM_{labor} + f_{maintlab} \times (\text{Maintenance cost})] \]

Operating costs: coal plant

Assume a similar cost structure (maintenance, labor, and admin & support labor costs) as for the oxygen plant.

Operating costs: power plant
The NETL report indicates that the total operating cost (fixed and variable) of a 555 MW plant is US$18 million per annum (2007 dollars). Assume that the operating cost is proportional to plant size.
Cost

Example 10: Cost Principles
Engineering economics:
How to compare process options with different capital and operational costs.
(Net Present Value, Internal Rate of Return, Payback Period)
Example of application of costing principles:
Marginal abatement cost curves, for CO$_2$ reduction

**MAC curves show:**
Marginal cost *per unit of CO$_2$ saved*, vs. amount of CO$_2$ saved; cost arranged from low to high.
Drawing up curve hence requires estimates of:
- cost *(per CO$_2$ saved)*, of each measure
- amount of CO$_2$ saved, for each measure
Example of (global) MAC curve

Global GHG abatement cost curve beyond business-as-usual – 2030

How much abatement is necessary?

Major categories of abatement opportunities

- Business as usual
- Energy efficiency
- Low carbon energy supply
- Behaviour change

Graph depicting the impact of different abatement measures over time.

Where do these costs estimates come from?
Capital costs and operational costs, expressed on common basis over life of project

Useful summary of equations:

\[ \text{NPV} = -C_S - C_T - C_D - C_E - \sum_{i=1}^{i=L} \frac{C_{S,i} + C_{T,i} + C_{D,i} + C_{E,i}}{(1 + d)^i} \]
\[ - \sum_{i=1}^{i=L+N} \frac{C_{D,MON,i}}{(1 + d)^i} - \frac{D_S + D_T + D_D}{(1 + d)^f} \]
\[ + \sum_{i=1}^{i=L} \frac{C_{S,i} + C_{T,i} + C_{D,i} + C_{E,i}}{(1 + d)^i} \]

(1)
Net present value:
Future costs and benefits expressed as present-day value
capital expenditure at 
start of project ... operating cost) in year i of project
discount rate
decommissioning 
costs at the end of 
the project life

\[
\text{NPV} = C_S - C_T - C_D - C_F - \sum_{i=1}^{L+N} \frac{C_D + C_F + C_D + C_F}{(1 + d)^i}
- \sum_{i=1}^{L+N} \frac{C_D + C_F + C_D + C_F}{(1 + d)^i}
+ \sum_{i=1}^{L} \frac{C_T + C_F + C_D + C_F}{(1 + d)^i}
- \sum_{i=1}^{L} \frac{C_T + C_F + C_D + C_F}{(1 + d)^i}
\]

(1)

decommissioning costs at the end of 
the project life
NPV: basis of cost-benefit analysis, e.g. of education

US Census Bureau, 2009 data

- Median annual income ($)
What is the discount rate?
The discount rate expresses the "time value of money".

The discount rate is "the rate, per year, at which future values are diminished to make them comparable to values in the present. Can be either subjective (reflecting personal time preference) or objective (a market interest rate)."

Funds required per annum to meet all future costs:
(Klemeš et al.)

\[
\text{CRF} = \frac{d(1 + d)^n}{(1 + d)^n - 1}
\]

\[-\text{NPV} \times \text{CRF}\]

\(d\): interest rate for repayment period
\(n\): total number of repayments
Capital investment: calculating loan repayment amounts
Similar to home mortgage:
Normally: fixed monthly repayment, covering interest and repaying loan ("principal")
⇒ Early in repayment period, less of payment goes towards repaying principal (and more to interest)
Monthly repayments (millions of $):
loan of $350M, 5% interest, 10-year period

Payment amount

Payment no.

Principal

Interest
Monthly repayments (millions of $):
loan of $350M, 10% interest, 10-year period

Payment amount
Payment no.
Principal
Interest

Monthly repayments (millions of $):
loan of $350M, 10% interest, 10-year period

Payment amount
Payment no.
Principal
Interest
Other cost comparison terms used:

Internal Rate of Return:
Discount rate which makes NPV=0
(Higher IRR ⇒ better project)

Payback period:
Length of time into project lifetime when integrated cash flow (including initial capital expenditure) becomes positive
(time value of money not taken into account)
Comparing alternative projects requires:
Estimate of capital costs
(e.g. from published correlations; suppliers)
Estimate of operating costs

*Both of these are directly related to mass and energy balances*
Different accuracies of capital estimates at different stages of project:

<table>
<thead>
<tr>
<th>Estimate Class</th>
<th>Level of Project Definition</th>
<th>Primary Characteristic</th>
<th>End Usage Typical purpose of estimate</th>
<th>Methodology Typical estimating method</th>
<th>Required Accuracy Range Typical variation in low and high range</th>
<th>Preparation Effort Typical degree of effort relative to last cost estimate of L</th>
</tr>
</thead>
<tbody>
<tr>
<td>Class 5</td>
<td>0% to 2%</td>
<td>Concept Screening</td>
<td>Capacity Tonnage, Symmetric Models, Adjustment, or Average</td>
<td>Li: 20% to -20%, Hi: 10% to 130%</td>
<td>1</td>
<td></td>
</tr>
<tr>
<td>Class 4</td>
<td>1% to 15%</td>
<td>Study of Feasibility</td>
<td>Equipment</td>
<td>Li: -15% to -30%, Hi: -20% to +50%</td>
<td>2 to 4</td>
<td></td>
</tr>
<tr>
<td>Class 3</td>
<td>10% to 40%</td>
<td>Budget Authorization, or Control</td>
<td>Scale Fixed Unit Costs with Assembly Line Items</td>
<td>Li: 30% to -20%, Hi: -15% to +50%</td>
<td>3 to 10</td>
<td></td>
</tr>
<tr>
<td>Class 2</td>
<td>30% to 70%</td>
<td>Control or Bid/Tender</td>
<td>Detailed Unit Cost With Detailed Take-Off</td>
<td>Li: -5% to -15%, Hi: 5% to +20%</td>
<td>4 to 20</td>
<td></td>
</tr>
<tr>
<td>Class 1</td>
<td>50% to 100%</td>
<td>Check Estimate or Bid/Tender</td>
<td>Detailed Unit Cost With Detailed Take-Off</td>
<td>Li: -5% to -15%, Hi: +5% to +15%</td>
<td>5 to 100</td>
<td></td>
</tr>
</tbody>
</table>

Example considered: “BF plus”

- high calorific value top gas
- electric power generation
- higher fuel injection rate
- colder blast with higher O₂
“BF plus”

Current status
- Recent similar approaches
  (electricity from gas turbines with BF top gas):
  ArcelorMittal Indiana Harbor;
  JFE Chiba works

Fundamental features
- colder blast $\Rightarrow$ small increase in fuel rate
- gas turbine plant highly capital intensive
“BF plus”

- Productivity 25% higher (high O₂ enrichment)
- Coke rate lower by 150 kg/THM
- CO₂ intensity lower by 250 kg/THM (with 300 kg CO₂/THM credit for electricity)
- Operating cost drivers:
  - coke savings; income from electricity

  (for increase in PCI rate from 150 kg/THM to 300 kg/THM)
Financial Model – Practical Work
Smelting Furnace Model – Practical Work
Techno-economic Modelling
Techno-economic Model

- A combination of
  - a financial model (simple or comprehensive)
  - with one or more technical models,
  - together with an optimiser (optional)
- Could perhaps be called a "techno-financial model".
- Used to model business cases while taking into account technical dependencies and constraints in the calculation of revenue, operational expenses and capital cost.
- Applications:
  - project feasibility studies,
  - pricing calculations (e.g. value-in-use),
  - financial planning,
  - scenario evaluations,
  - etc.
Financial Model

- A mathematical model to describe the behaviour of a financial entity (e.g. company, department, project, person, etc.).
- Based on accounting and financial principles.
- Applications (same as techno-economic):
  - project feasibility studies,
  - pricing calculations (e.g. value-in-use),
  - financial planning,
  - scenario evaluations,
  - etc.
General Ledger (GL)

- Forms the core of the financial model.
- Central repository for all financial transactions.
- Basis for:
  - balance sheet,
  - income statement,
  - cash flow,
  - and other reports.
  
  As a function of time (if more than one period is simulated).
- All important financial metrics can be calculated from the content of the general ledger. E.g. IRR, NPV, EBIT, EBITDA, profit margin, etc.

<table>
<thead>
<tr>
<th>Date</th>
<th>Description</th>
<th>Account</th>
<th>Debit</th>
<th>Credit</th>
</tr>
</thead>
<tbody>
<tr>
<td>2023/01/01</td>
<td>Long term loan</td>
<td>Liability, Long Term Loan</td>
<td>USD 400,000.00</td>
<td></td>
</tr>
<tr>
<td>2023/01/01</td>
<td>Loan interest</td>
<td>Expenses, Loan Interest</td>
<td>USD 3,000.00</td>
<td>USD 3,000.00</td>
</tr>
<tr>
<td>2023/02/01</td>
<td>Loan interest</td>
<td>Liability, Long Term Loan</td>
<td></td>
<td>USD 3,000.00</td>
</tr>
<tr>
<td>2023/02/01</td>
<td>Loan repayment</td>
<td>Liability, Long Term Loan</td>
<td>USD 100,000.00</td>
<td>USD 100,000.00</td>
</tr>
<tr>
<td>2023/02/01</td>
<td>Loan repayment</td>
<td>Liability, Long Term Loan</td>
<td>USD 100,000.00</td>
<td>USD 100,000.00</td>
</tr>
</tbody>
</table>

Make sure to check the accuracy and completeness of the entries.
Debits and Credits

- The GL uses the double entry book keeping system.
- Each transaction is recorded with two entries (a debit and a credit) in the GL.
- The source account of a transaction is usually credited, and the destination account debited.

<table>
<thead>
<tr>
<th></th>
<th>Debit</th>
<th>Credit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Asset</td>
<td>Increase</td>
<td>Decrease</td>
</tr>
<tr>
<td>Liability</td>
<td>Decrease</td>
<td>Increase</td>
</tr>
<tr>
<td>Income/Revenue</td>
<td>Decrease</td>
<td>Increase</td>
</tr>
<tr>
<td>Expense</td>
<td>Increase</td>
<td>Decrease</td>
</tr>
<tr>
<td>Equity/Capital</td>
<td>Decrease</td>
<td>Increase</td>
</tr>
</tbody>
</table>
Balance Sheet

Based on the accounting equation:

\[ \text{Assets} = \text{Liabilities} + \text{Owner's Equity} \]

or

\[ \text{Owner's Equity} = \text{Assets} - \text{Liabilities} \]

Used to display financial state of a business at a specific point in time.
**Income Statement**

Based on the equation (simplified): Net Income = Income – Expenses

<table>
<thead>
<tr>
<th>Item</th>
<th>2013</th>
</tr>
</thead>
<tbody>
<tr>
<td>Product Sales</td>
<td>USD 10 000 000</td>
</tr>
<tr>
<td>Total</td>
<td>USD 10 000 000</td>
</tr>
<tr>
<td>Net Sales</td>
<td>USD 10 000 000</td>
</tr>
<tr>
<td>Less: Expenses</td>
<td>USD 1 000 000</td>
</tr>
<tr>
<td>Total</td>
<td>USD 1 000 000</td>
</tr>
<tr>
<td>Gross Profit</td>
<td>USD 9 000 000</td>
</tr>
<tr>
<td>Less: Operating Expenses</td>
<td>USD 1 000 000</td>
</tr>
<tr>
<td>Total</td>
<td>USD 1 000 000</td>
</tr>
<tr>
<td>Net Profit</td>
<td>USD 8 000 000</td>
</tr>
</tbody>
</table>

Used to indicate the business’s income, expenses and profitability

*Source: SAIMM Pyrometallurgical Modelling Workshop 2014*
Financial Model

Use a mathematical model of the business to describe business activities by generating appropriate financial transactions. One activity may result in a large number of transactions. For example, a long term loan:

- Obtain long term loan: Credit Loan -> Debit Bank
- Interest on loan: Credit Loan -> Debit Loan Interest
- Pay loan interest: Credit Bank -> Debit Loan
- Pay loan capital: Credit Bank -> Debit Loan

Other activities:

- Asset acquisition (payment, depreciation, write-off)
- Production expenses
- Product sales
- Income tax
Why use a general ledger as basis?
- Standardised, simple integration of technical model results.
- Rich, standardised reporting.
- Clear communication with financial and business personnel.
Modularity vs. Complexity

- Separate spreadsheets for the different models. Isolate complexity to individual models, limiting combined complexity.
- Communication via model parameters and transactions. Simplify interaction between models.
- Technical models produce figures to generate GL transactions.
- Financial model reads results from technical models.
- Technical models read parameters from financial models.
Integrating a Smelter Model into a Business Model

Consider an ilmenite smelter that will form part of a large heavy minerals project. The project has a comprehensive financial model to simulate its future performance, but needs a separate smelting furnace model to provide realistic consumption and production figures.

- The financial model exists as an Excel spreadsheet, and uses a general ledger to capture all transactions.
- A smelting furnace model exists in a separate spreadsheet.
- The two models can be combined into a single spreadsheet, but at the risk of increasing complexity, reduced maintainability and a larger risk of errors.
- The two models are maintained by separate individuals with focused and different knowledge and skill sets.

See the provided spreadsheets as an example.