Introduction
The smelting and refining operations associated with non-ferrous metal recovery, especially from sulphide raw materials, produce process off-gas at temperatures above 1300°C. The hot off-gas contains concerning quantities of SO₂ and a substantial amount of entrained dust particles of which some may occur in the molten or semi-molten phase. Therefore the need arises for adequate treatment of the gas in order to recover energy and dust while meeting process and environmental requirements.

Synopsis
The waste-heat boiler is used within the Sulphide flash smelting process as the main dust and energy recovery unit. The large volume of off-gas discharged from the flash smelter is at a very high temperature (1350°C) and contains a significant dust load that subjects the downstream waste-heat boiler to tough and demanding conditions. The boiler cavity is especially prone to dust accretions, fouling, and corrosion caused by accumulation of molten particles and precipitation of sulphuric acid.

Computational fluid dynamics (CFD) is applied within a qualitative study to model the flow and heat transfer distribution throughout the waste-heat boiler. The commercial CFD package, Fluent 6.2.16, was applied to a modified waste-heat boiler (23 m × 11 m × 5.4 m) within the Outokumpu flash smelting process.

This investigation focuses on the geometric modifications to the typical boiler design, which includes elevation of the ceiling, placement of flow-obstructing baffles and radiation plates parallel within the flow path. Also investigated were various boiler operating conditions such as the circulation of process off-gas, air leakage from the dust discharging hoppers and variation in inlet gas composition.

The geometric modifications had the desired effect of increasing the volumetric utilization and therefore enhancing heat transfer between the boiler surface and the gas stream and dust segregation. Introducing circulated off-gas at a rate of 20 m/s and at a 45° angle to the front of the waste boiler further enhanced cooling while reducing the high impact of the furnace-uptake gas-stream on the boiler ceiling. The placement of radiation plates was found to be very effective in enhancing the heat transfer surface and distributing gas flow within the boiler. These results present recommendations towards an improved waste-heat boiler design.

Keywords: flash smelting, waste-heat boiler, CFD simulation, off-gas cooling.

The development of the Outokumpu flash smelting process in 1949 presented the horizontal waste-heat boiler for reduction of waste-heat losses and recovery of flue dust, which, today, is still the proven and dominating technology regarding smelter off-gas handling. The gas-cooling step, of which the waste-heat boiler is the principal component, has the most extreme operating conditions due to high gas temperature and high dust load, its is thus a mayor bottleneck and opportunity for process optimization. The off-gas handling unit also contributes substantially to the main investment cost, up to 25 to 50 per cent, of a smelter. It is therefore paramount that the design of the gas-handling solution must incorporate an in-depth evaluation and understanding of the process and equipment operation.

Considerable development of the waste-heat boiler has taken place since its introduction. These developments include changes in geometry, flow characteristics, cleaning technology and design details. Various modelling attempts have been made in order to improve the understanding of the specific process requirements. Prototyping and online measurements have provided some knowledge, but due to expense and alteration difficulties have fallen short of providing efficient results.

Computational fluid dynamics (CFD) modelling provides a powerful tool for evaluating designs based on virtual computer prototyping and was used within the present study to simulate the flow and heat transfer through the boiler space in order to identify...
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more efficient boiler designs. Such a design would include geometry and operating conditions that will minimize the problems encountered within the general waste-heat boiler, e.g. elimination of dead areas, ineffective heat transfer and mixing, dust segregation and

The study presents a qualitative approach for evaluating the modelling results but does, however, fall short of verification through data comparison from the actual system. Care is, however, taken within the modelling outcome to ensure numerical validation through the establishment of grid independence and sound convergence. The merits of this revised study are further identified through the close comparison to previous modelling studies.

The commercial CFD package, Fluent® version 6.2.16 was used for simulating the flow and heat transfer phenomenon within a modified design of the conventional waste-heat boiler. The conventional waste-heat boiler is characterized by a straight roof stretching from the boiler inlet to the outlet and a completely empty interior. The modified design investigated included an elevation of the front part of the boiler ceiling by 1.4 m and the placement of radiation plates and a sunken baffle suspended from the ceiling to enhance heat transfer and improve residence time within the waste-heat boiler. Furnace uptake angles of 60°, 45° and 30° were investigated in the light of the impact on the boiler structure and the most efficient gas stream produced within the boiler. The effect of operating conditions inherent in the Outokumpu Flash Smelting Process were also considered with the main focus being circulation of the process off-gas, air leakage from the dust hoppers and variation in the inlet process gas composition. The SO₂ concentration was of particular interest.

The waste-heat boiler in the copper flash smelting process

The modified waste-heat boiler design includes a front radiation section and a smaller convection section (see Figure 1). The radiation section receives the hot, dust-laden off-gas from the uptake shaft and rapidly cools the hot gas and recovers dust to a satisfactory standard before being handled by the convection section. The boiler consists of membrane walls, which along with the radiation plates placed within the radiation section and the tube banks placed within the convection section, are cooled by circulation of saturated steam at high pressure. Four rows of radiation plates are installed to provide additional heat transfer surfaces. Energy is recovered from the superheated steam while the off-gas is cooled from an entering 1200–1350°C to approximately 350°C before it is allowed to enter the proceeding electrostatic precipitator. Approximately two-thirds of the entering dust is recovered by the waste-heat boiler.

Conditions of concern within the boiler require an optimum design so as to limit its effect on the disruption of the continuous process. The conventional straight-roof boiler produces a gas jet stream along the boiler ceiling that presents poor utilization of the boiler space due to the limited residence time for cooling and dust segregation. It was proposed to elevate the front ceiling of the radiation section and to place a flow-obstructing baffle within the main flow path to enforce circular motion and increase the residence time for heat transfer and dust segregation.

Of high concern are the reactions occurring within the boiler. The dust sulphating reactions, reactions between the metal oxides and SO₂, are highly exothermic and must be completed before entry to the convection section. The oxidation of SO₂, also an exothermic reaction, presents the possibility of sulphuric acid formation within the boiler that could lead to serious fouling effects. The maximum reaction temperature for SO₂ oxidation is within the range 500–600°C, while H₂SO₄ condensation is expected at temperatures lower than 200°C. Therefore a temperature window is presented within which the boiler should be operated. The gas must also be rapidly cooled in the radiation section to below 700°C to prevent molten particles adhering to the boiler surfaces and tube banks in the convection section that could lead to dust accretions.

The air leakage from the dust hoppers as a result of the lower pressure created within the waste-heat boiler is an inevitable concern since unloading and conveying of the captured dust have to occur during operation. The air leakage could impose problems due to the low temperature and high O₂ content, hence providing the potential for SO₂ oxidation and fouling.

The modelled waste-heat boiler is designed to handle the off-gas from a furnace uptake at a flow of 37000 Nm³/h and temperature of 1350°C. The effect of two circulating off-gas

[Diagram: Adapted schematic representation of the modelled waste-heat boiler]
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rate, 10000 Nm$^3$/h and 18000 nm$^3$/h at a temperature of 300°C, were investigated. The off-gas was introduced at an inclined slot above the radiation section. Air leakage amounted to 3000 Nm$^3$/h for the radiation section and 2000 Nm$^3$/h into the convection section at ambient conditions.

Modelling methodology

Solution domain
The solution domain is established by creating a 3D geometry representing the 25 (L) x 5.4 (B) x 11 m (H) waste-heat boiler and fitting it with an appropriate grid and boundary conditions. Gambit 2.2, the pre-processing package for Fluent 6.2.16, was used to generate the geometry and mesh the computational domain that is exported to the Fluent 5/6 solver. The front, radiation section of the boiler was modelled first, followed by the full boiler geometry once the model specifications had been established.

In an attempt to improve the conventional waste-heat boiler design, four rows of equally spaced radiation plates of various lengths were suspended from the radiation section ceiling. Four plates were placed at the gas entry region and eight were placed on both sides of the centre baffle and at the outlet of the radiation section. The boiler geometry further included two dust hoppers for the radiation section and six for the convection section, while off-gas circulation is introduced through a rectangular slot on the front elevated roof incline. In the convection section, the actual tube banks were simplified by five rows of cooling plates.

The 3D computational domain was meshed mostly with tetrahedral elements due to the rigid and abrupt nature of the space left for gas-flow. Various grid refinements were considered in a grid independence study that revealed a computational domain containing 525, 250 active mesh elements of very low skewness to be adequate for capturing the desired property characteristics.

Model specifications
The technique of CFD involves the numerical solving of a collection of conservation equations describing the balance between the various factors influencing the specific dependent variables while being coupled with empirical models that have been developed in an attempt to represent the physical phenomena that attribute to these influences. The modelling of the waste-heat boiler is dependent on such empirical models for including the effects of turbulence and radiation heat transfer. Fluent provides a variety of physical models of which the most adequate are chosen for representing the system of interest.

The steady state convection and diffusion equations for the dependent variables, represented by a generalized Equation [1], are solved by a segregated solver, implying sequential solution of the model equations. This solver is selected for being more appropriate for solving incompressible or mildly compressible flows as opposed to a coupled solver, which is more suited for calculating high-speed flows and not true for this model.

\[ V \cdot \left( \rho \nabla \phi \right) = V \cdot \left( \left[ \nabla \phi \right] - S \right) \]  

For this equation:
- \( \phi \) : The dependent flow variable representing the velocity component, temperature, turbulence kinetic energy or its dissipation rate, radiosity.
- \( \nabla \phi \) : Velocity vector.
- \( \rho \) : Density of the fluid phase.
- \( S \) : General source term relevant to the variable \( \phi \). 

Turbulence modelling

The present version of Fluent is equipped with a large selection of models for describing turbulence phenomena. Choice had fallen on the standard k-ε model and the RNG-turbulence model for representing the effect of turbulence. The standard k-ε model is a semi-empirical code that is based on the model transport equations for turbulence kinetic energy \( \left(k\right) \) and the turbulent kinetic energy dissipation rate \( \left(\epsilon\right) \) whereas the RNG-based k-ε model is derived from the instantaneous Navier-Stokes equations using a mathematical technique referred to as “renormalization group” (RNG).

The major differences between these models are their method for calculating the turbulent viscosity, the turbulent Prandtl numbers, turbulent generation and dissipation terms and the turbulent flow parameters that are employed. The standard k-ε model is, however, preferred due to its robustness, economy of computational effort and reasonable accuracy for a wide range of turbulent flow, while the RNG-model requires high computational time but does represent swirling motion to a higher accuracy. These models were compared based on the outcome when incorporated in a similar model set-up.

Treatment of the near-wall regions

Turbulence modelling does fall short of describing turbulence at the near-wall regions due to the large gradient in the solution variables and low values for the Reynolds turbulence number. For this reason wall functions are developed to prevent the use of a computationally expensive high-resolution mesh at these regions. Standard type wall functions were selected to represent the near-wall regions since non-equilibrium wall functions are relevant only for
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complex flows involving separation, reattachment and severe pressure gradients with the mean flow and turbulence changing rapidly. Fluent's enhanced wall functions incorporate a laminar combined with the logarithmic (turbulent) law-of-the-wall function, which, due to extreme computational expense, is not considered for the modelling of the waste-heat boiler.

As required for application of wall functions, the dimensionless distance from the wall ($y^+$) was monitored to ensure its value remains within the valid range of 30 to 300.

Boundary conditions for the standard and RNG k-ε models

The chosen wall functions automatically make provision for the boundary conditions of $k$ and $ε$ at the wall regions; however, user inputs for $k$ and $ε$ are required for the inlet boundary conditions. The use of experimental or previously determined values is preferred. However, because no such information was available, first order approximations were used. To estimate the inlet boundary condition, relationships that specify the turbulence quantities in terms of computable quantities, e.g. turbulence intensity, hydraulic diameter and turbulence length scale, were applied.

The turbulence intensity, $I$, which is the ratio of root-mean-square of velocity fluctuations to the mean flow velocity, was obtained by:

$$I = 0.16 \left( \frac{Re_{in}}{100} \right)^{1/8}$$

[2]

The hydraulic diameter, $D_H$, and average free stream velocity, $u_{avg}$, were used to determine the Reynolds number, $Re_{in}$. For fully developed duct flows, as in the case for upward flow within the uptake-shaft, $D_H$ can be considered equivalent to the characteristic length of the inlet.

The turbulent kinetic energy was obtained from:

$$k = \frac{2}{3} \left( u_{avg} \right)^2$$

[3]

and $ε$ was estimated using the relationship:

$$ε = C_ε \frac{k^{3/2}}{l}$$

[4]

where the value of $C_ε$, an empirical constant specified in the turbulence model, is approximately 0.09. The turbulence length scale, $l$, was estimated by an approximate relationship between $I$ and the characteristic length, $L$:

$$l = 0.07L$$

[5]

Radiative heat transfer model

Five radiation models are provided within Fluent 6.2.16 computational range. The P-1 radiation model was chosen to model the radiation heat transfer for the present study, since it allows the effect of scattering to be incorporated in the modelling and since the optical length within the waste-heat boiler, approximated by Equation [6], is below a 3 m criterion for eliminating other potential models:

$$s = (a + σ_V) \frac{V}{A}$$

[6]

The P-1 model is able to include the effect of particulate medium at the expense of thorough modelling of the effect of scattering by gas. However, due to the large excess of gas compared to particulates, it was considered a sound approximation to exclude the modelling of gas-particulate scattering but to make provision by applying a modified average scattering coefficient.

The absorption, $a$, and scattering, $σ_V$, coefficients of the radiative medium are the only input properties required by the P-1 model. These were calculated as the weighted average of the components, as presented further on.

Physical properties and heat transfer parameters

The required physical properties are well described in literature and well presented by the previous modelling study by Yang. The composition of the furnace uptake off-gas to be treated by the waste-heat boiler was obtained from Yang and presented in Table I.

As indicated, SO$_2$ and N$_2$ comprise the majority of the process off-gas and were therefore used as a basis for deriving the property expressions by means of weighted average. The ideal gas law and kinetic theory of gasses, assuming negligible volume and no interaction between molecules, were used to estimate the gas mixture density while the temperature dependent properties were represented through polynomial expressions.

For simplification and in an attempt to reduce computational effort, the physical property expressions were reduced to a constant average through integration over the waste-heat boiler operating temperature range (300 K to 1400 K). The property relationships that were obtained are presented in Table II.

The absorption and scattering coefficients were the only requirements for radiation modelling. The absorption coefficient was calculated by incorporating the effects of the main absorption components, SO$_2$, CO$_2$ and H$_2$O, in the gas mixture. The mathematical expression presented in study by Hahn was used to relate the total gas emissivity to the gas absorption coefficient, specifically derived for the gas mixture in the sulphide flash smelting process.

$$a = \left[ \ln(1 - ε) \right] / l_m$$

[7]

An absorption coefficient of 0.54 was calculated accordingly. For the above expression $ε g$ represents the total gas emissivity and $l_m$ the mean beam length, which in turn was estimated from the relation below where $V$ and $A$ denote the volume and area of the waste-heat boiler radiation section respectively.

$$l_m = 3.5(V/A)$$

[8]

Table I

<table>
<thead>
<tr>
<th>Process gas composition for the modified waste-heat-boiler</th>
</tr>
</thead>
<tbody>
<tr>
<td>Component</td>
</tr>
<tr>
<td>SO$_2$</td>
</tr>
<tr>
<td>CO$_2$</td>
</tr>
<tr>
<td>H$_2$O</td>
</tr>
<tr>
<td>O$_2$</td>
</tr>
<tr>
<td>N$_2$</td>
</tr>
</tbody>
</table>
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The total gas emissivity was computed by the weighted average of the emissivities of the absorbing gas components. These emissivities were obtained from Hottel and were averaged over the operating temperature range. The resulting emissivities are presented in the Table III.

As stated, the effect of scattering brought about by the particulate medium was incorporated by a modified gas scattering coefficient. The study by Hahn provided the relationship to calculate the scattering coefficient as the sum of the individual particle contributions in a unit volume:

$$\sigma_s = \sum_j K_j = \sum_j \eta_j d_j$$

For this relation $\eta_j$ is the particle scattering efficiency, $\eta_j$ represents the particle density number, while $d_j$ is the particle diameter of the $j$th size fraction. A similar expression to the above equation was used to include the particulate contribution in the total absorption coefficient.

**Boundary conditions**

The boundary conditions assigned during the preprocessing stage using the package Gambit 2.2 were defined in the Fluent 6.2.16 solver. The specifications of these boundary conditions are described:

**Velocity inlet (furnace uptake)**

A horizontal inlet velocity of 15 m/s was allocated normal to the vertical boundary allocated at the bottom of the furnace up-take shaft that was included in the computational model. The value is similar to that applied by Yang and represents the volumetric flow rate of 10000 Nm$^3$/h. The temperature of the uptake was taken as 1623 K (1350°C). The temperature difference of the uptake plates very small. This assumption is partially justified by the fact the diatomic gasses show no absorption of radiation energy while very little CO$_2$ gas is present to have an effect on the energy distribution within the boiler.

**Pressure outlet (radiation section outlet)**

The outlet of the radiation section was assigned an operating pressure of 0.95 bar (- 5066 Pa gauge pressure). This condition was used for representing actual operation of the boiler since it is maintained at slight under pressure to maintain gas flow and prevent excessive air leakage from the dust hoppers.

**Velocity inlet (off-gas circulation)**

The off-gas was reintroduced to the radiation section at a rate of 12 m/s or 20 m/s, relating to the volumetric rates of 10000 and 18000 Nm$^3$/h respectively. These rates were assigned normal to the rectangular inlet slot at a temperature of 300°C. The properties of the circulating gas were defined the same as the process gas mixture discussed previously.

**Velocity inlet (air leakage)**

Air leakage was introduced by defining an inlet velocity of 0.33 m/s (relating to 3000 Nm$^3$/h for the radiation section and 2000 Nm$^3$/h for the convection section of the waste-heat boiler) from the bottom dust hoppers at a temperature of 300 K. The air entering through these boundaries was assigned properties of air at ambient conditions.

**Wall (boiler walls, roof and radiation plates)**

The boiler walls and radiation plates were defined under radiation boundary conditions and not wall flux conditions. This allowed specification of a surface emissivity of 0.78, typical of carbon steel and a wall temperature of 573 K (300°C). A uniform temperature boundary condition for the plates would imply that the temperature difference of the high-pressure steam flowing through the tubes within the plates very small. This assumption is partially justified by the high actual flow rates of the steam.

**Assumptions and justification**

The most important assumption made during the modelling of the waste-heat boiler are identified and discussed:

- Neglecting the reaction heat associated with the dust sulphating and SO$_2$ oxidation reactions will result in an outlet gas temperature to be lower. The assumption is required due to the considerable computational extent of including reacting species. However, the model outcome will provide a good indication as to the general heat distribution within the boiler.
- The absence of particulate media, also omitted to reduce computational expense, will also lead to a slight under prediction of the gas temperature. Compensation is made through an adapted scattering and absorption coefficient stated previously.
- The assumption of a binary gas inlet composition is justified by the fact the diatomic gasses show no absorption of radiation energy while very little CO$_2$ gas is present to have an effect on the energy distribution within the boiler.

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### Table II: Thermophysical property relationships developed to describe the gas mixture

<table>
<thead>
<tr>
<th>Physical property</th>
<th>Formula</th>
<th>Constant average (300–1400 K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Density (kg/m$^3$)</td>
<td>$\rho = 0.005106 T^2$</td>
<td>—</td>
</tr>
<tr>
<td>Specific heat (J/kg.K)</td>
<td>$\epsilon_a(T) = 5.01 \times 10^{-3} T^3 - 2.71 \times 10^{-1} T^2 + 0.54187 + 597.153$</td>
<td>878.09</td>
</tr>
<tr>
<td>Viscosity (Ns/m$^2$)</td>
<td>$\mu(T) = 9.51 \times 10^{-3} + 5.1046 \times 10^{-5} T - 1.994 \times 10^{-7}$</td>
<td>3.968 x 10$^{-6}$</td>
</tr>
<tr>
<td>Thermal conductivity [W/mK]</td>
<td>$k(T) = -1.12 \times 10^{-8} + 4.1046 \times 10^{-1} T^2 + 0.54187 T + 0.003$</td>
<td>0.042</td>
</tr>
</tbody>
</table>

### Table III: Component and total gas mixture emissivities

<table>
<thead>
<tr>
<th>Component</th>
<th>Total</th>
<th>Emissivity</th>
</tr>
</thead>
<tbody>
<tr>
<td>CO$_2$</td>
<td>0.15</td>
<td>0.08</td>
</tr>
<tr>
<td>SO$_2$</td>
<td>12.3</td>
<td>0.08</td>
</tr>
</tbody>
</table>
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Convergence monitoring

The computational intensity of this modelling attempt requires close monitoring of the model residuals and taking a stepwise approach for promoting and enhancing convergence. The solution criteria for the first couple of iterations were set to a first-order upwind scheme, the simplest advection scheme for converting the governing equations to control-volume-based algebraic equations. Since the computational domain contains a large number of tetrahedral mesh elements, the first-order upwind scheme would not be an accurate representation. To acquire representative initial values for the mesh and so promote convergence, the second-order upwind scheme was activated at later stage. Furthermore, the under relaxation factors for the model equations were reduced during the initial stage of the simulation but restored later in the iteration process. Some convergence difficulties were overcome by disabling the diffusion energy source, as specified in the Fluent User’s Guide.

Simulation results

The effect of geometric modifications

The effect of various furnace uptake angles was tested through simulating a waste-heat boiler geometry containing a 60°, 45°, and 30° furnace uptake shaft. An uptake angle of 45° was found to be the optimum angle for introducing the off-gas to the waste-heat boiler. A larger uptake angle, 60°, caused high impact of the inlet gas stream on the front ceiling and higher turbulence in the front part of the waste-heat boiler radiation section. High impact on the boiler ceiling should be prevented from rupturing of the boiler roof while excessive turbulence in the boiler makes it prone to fouling. A 45° angle revealed an optimum utilization of the boiler cavity and will therefore provide maximum contact for the process off-gas with the suspended radiation plates in the entry region. Such an angle will also provide satisfactory residence time for dust particles to segregate while allowing minimum potential for dust accretions and stress on the boiler structure. Similar findings were observed by Yang, who stated 47.6° to be the optimum angle for directing the process off-gas to the boiler interior.

The flow-profiles showed that the geometric modifications to the conventional waste-heat boiler design, elevating the front part of the radiation section ceiling and suspending a sunken baffle halfway, revealed a great improvement in the volumetric utilization and outflow gas temperature. The conventional, straight-roof boiler resulted in a poor WHB volumetric utilization due to the gas stream passing straight through the boiler having no swirling motion to utilize the lower boiler cavity. A higher temperature and dust load will result to the convection section.

The elevated ceiling at the front part of the boiler had the effect of reducing the impact on the roof and enhancing circular motion of the gas stream, thus improving residence time. The sunken baffle further enhanced downward circular motion, resulting in an S-shaped flow stream through the radiation section, further improving residence time. The enhanced residence time will allow more effective heat transfer to the radiation plates and boiler membrane walls.

The effect of including radiation plates

Gas-flow

Suspending radiation plates from the ceiling of the radiation section further reduced the impact of the entering gas-stream on the boiler ceiling and the sunken baffle and therefore further preventing undesired corrosion and fouling. It was found that the radiation plates distributed the off-gas stream more evenly through the boiler cavity and eliminated excessive turbulence at an early stage. By preventing abrupt
changes in the motion of the gas-stream, especially in the cooler part of the boiler, possible precipitation of sulphuric acid and therefore fouling will be prevented.

Having the temperature and gas-flow distribution higher in the front part of the waste-heat boiler is considered better operation when having a high temperature and a high dust laden gas-stream entering the convection section where the exposed tube bundles will be vulnerable to fouling.

The relatively stagnant zones detected near the dust hopper outlets and in the bottom part of the radiation section are considered advantageous for dust particles to agglomerate and segregate. The cooler stagnant area in the bottom of the radiation section prior to the convection section is especially preferred since it will allow dust particles to settle before being carried over into the convection section.

Figure 5, a horizontal intersection at the upper part of the radiation section, shows a symmetrical horizontal swirling motion moving from the centre towards the outward boiler wall. This is considered advantageous for preventing dust accretions at the boiler wall and corners due to the high flow and elimination of stagnant areas. The model without radiation plates revealed flow to be absent or very low at the near-wall regions, which would allow potential for dust accretion.

The model without radiation plates resulted in a much higher residence time in the bottom, cooler part of the radiation section when compared to the model where plates were suspended from the boiler roof. Too high residence time in this region will result in high potential for SO₂ oxidation, especially due to the air leakage from the dust hoppers. The presence of radiation plates reduced the residence time in the bottom part of the boiler while increasing the flow distribution in the top part of the boiler, as stated previously.

**Temperature distribution**

The placement of radiation plates revealed an average decrease of 100°C at the outlet boundary of the radiation section compared to the waste-heat boiler where radiation plates were omitted. The very advantageous faster transition between the temperatures 600°C to 500°C was also observed for the model including the radiation plates. This is desired operation for preventing SO₂ oxidation and hence reducing the potential for acid formation. Temperatures within this range follow a narrow distribution from the bottom part of the boiler towards the outlet, therefore avoiding exposing large areas to these temperatures.

Figure 4b depicts the primary dissipation of radiative energy to be in the front part of the radiation section of the waste-heat boiler. This clearly justifies the placement of
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plates in this region justifiable. However, a low radiation flux at the outlet region and cold region behind the sunken baffle indicate that the placement of radiation plates, especially in a high concentration, in this region is not necessary.

The temperature distributions between the first two rows of radiation plates and at the outlet section for the modified waste-heat boiler design were monitored and are presented by Figure 6.

Figure 6 shows the temperature above the centreline in the front part of the radiation section to be well above the SO$_2$ oxidation temperature range (above 600°C or 873 K). It can also be seen that the higher temperatures are concentrated in the centre of the top half of the boiler. The temperature below the roof (average 900 K) is still within the preferred range and below a temperature where dust will be present in molten form. The incident radiation flux is also largely concentrated within the centre of the elevated roof, making the placement of radiation plates within this region a good design.

Off-gas circulation

Off-gas is circulated with the intention of reducing the impinging effect on the boiler ceiling by suppressing the inlet gas-stream before the sunken baffle. This effect was observed when introducing off-gas at the inclined angle at the front of the radiation section upper section. It was observed that the reintroduction of cooler off-gas placed more duty on the boiler walls due to the inlet gas stream being forced towards the side walls and sunken baffle. However, gas cooling within the radiation section was found to be enhanced and the stagnant flow zone behind the sunken baffle slightly eliminated. These are considered good operating conditions.

An off-gas flow rate of 20 m/s was found to be the most effective rate for introducing the circulated off-gas. A lower circulated gas entry rate of 12 m/s revealed very little impact on the off-gas stream and little cooling effect in the front part of the boiler. Higher circulating off-gas flow rates, as modelled by Yang\textsuperscript{6}, of up to 60 m/s are not considered effective operation due to the reduction in the duty of the radiation plates while the off-gas stream is forced to the bottom section where dust is preferred to segregate. Stagnant areas behind the sunken baffle were also observed to worsen for higher circulating off-gas rates.

Air leakage

It was noted that the bottom section of the boiler is brought to a considerably lower temperature when including the effect of air leakage. The outlet gas at the radiation section was found to be an average 34°C cooler when including air leakage from the dust hoppers. The effect of air leakage, however inevitable, is not beneficial waste-heat boiler operation. The cooler, oxygen rich, air entering at the bottom subject the boiler to hazardous SO$_3$ formation and increases the potential for dust sulphating at the lower parts. There is concern about possible acid condensation and eventual hazardous dust accumulation. For this reason spring hammers are placed in these regions to prevent excessive build-ups and prolong the need for maintenance. Similar observations were made by Yang\textsuperscript{6}.

Variation in inlet concentration

SO$_2$ is the most important absorbing-emitting component of the entering off-gas stream. For this reason considerable change in the heat duty placed on the boiler was observed when altering the SO$_2$ concentration of the entering gas. The heat duty of the boiler was increased when the SO$_2$ concentration was increased. The high absorption coefficient of SO$_2$ is responsible for the gas-stream maintaining its energy state for longer and therefore leading to higher observed temperatures, especially in the radiation section. A high entering SO$_2$ concentration is regarded as concerning operation due to the high heat duty placed on the waste-heat boiler structure.

The potential for SO$_3$ formation increases according to the increase in SO$_2$ concentration. With higher SO$_2$ in the gas stream the chances for dust sulphating and acid condensation in the cooler parts of the boiler are radically increased, especially in the convection section. The SO$_2$ composition used in the simulation, 43.5%, is considered efficient since the heat transfer and temperature distribution within the waste-heat boiler was found to be effective and within a safe heat load.

Heat transfer efficiency and distribution

Radiative heat transfer was found to be approximately 83 to 93 per cent of the total mode of heat transfer to the boiler surfaces, therefore validating the need to include a radiation section within the waste-heat boiler design. It was found that the second row of radiation plates was subjected to the largest heat transfer duty, which along with heat transfer to the first row, substantiates the need for placement of plates in the front part of the boiler.

Overall, it was computed that the heat transferred to the radiation plates amounted to an average of 22% of the total heat transferred to the boiler surfaces. The load distribution among the different rows of radiation plates is presented in Table IV, showing the highest amount of heat to be absorbed by the second row of plates. This is considerably lower than the percentages reported by Yang\textsuperscript{6}, who recorded values of 40 to 50%. The heat associated with the dust sulphating and SO$_2$
oxidation reactions were not taken into account and are considered to be the reason for predicting a lower heat transfer rate.

**Sensitivity analysis**

**Grid independence**

As stated previously, the grid used was proven independent of further refinement since no change in the outcome was observed when the number of elements was doubled.

**Effect of different turbulence models**

The standard k-ε turbulence model was used for most of the simulations. The RNG k-ε turbulence model provided convergence difficulties and poor convergence was reached when this model was used.

The standard and RNG k-ε models were compared based on the turbulent viscosity, Figures 8. The standard k-ε model predicted high turbulence in the region of the uptake shaft and in the upper part of the entry region. The RNG model is more accurate in predicting swirling motion. However, since the swirling brought about in the gas stream is wide and spacious and not small or abrupt, the standard k-ε model was considered adequate for modelling the turbulence. Computational time was therefore saved at the risk of a slightly lower degree of accuracy.

**Effect of the absorption coefficient within the radiation model**

High sensitivity to the gas absorption coefficient was observed. A higher temperature was observed in the front part of the boiler when a small absorption coefficient was applied due to the high energy release in this region since the gas is not able to maintain its energy state.

The absorption coefficient could therefore largely affect the outcome of the simulated results and therefore the design of the boiler. Yang reported the choice of the SO2 absorption coefficient to be a large error source in the heat transfer modelling of the boiler. This is further confirmed by the sensitivity analysis for the SO2 concentration. The assumption of a constant gas emissivity, may further lead to errors since temperature differences of up to 700°C can be achieved within the boiler and could influence the emissivity which is temperature dependent.

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**Table IV**

**Percentage of the total heat transfer distribution among the radiation plates**

<table>
<thead>
<tr>
<th>Simulation</th>
<th>Total (W)</th>
<th>Row 1</th>
<th>Row 2</th>
<th>Row 3</th>
<th>Row 4</th>
</tr>
</thead>
<tbody>
<tr>
<td>20% SO2 concentration in off-gas</td>
<td>-14285483</td>
<td>4.56</td>
<td>13.40</td>
<td>2.71</td>
<td>1.37</td>
</tr>
<tr>
<td>40% SO2 concentration in off-gas</td>
<td>-14858164</td>
<td>4.80</td>
<td>13.54</td>
<td>2.75</td>
<td>1.40</td>
</tr>
<tr>
<td>60% SO2 concentration in off-gas</td>
<td>-15606092</td>
<td>4.83</td>
<td>14.00</td>
<td>2.89</td>
<td>1.41</td>
</tr>
</tbody>
</table>
Computational fluid dynamic modelling of a waste-heat boiler

Unfortunately the emissivity and absorption coefficients could not be validated with actual temperature measurements but a compromise is made through the assumption of omitting the energy contribution due to the sulphating reactions. The temperature profiles that were obtained compared fairly with those obtained by Yang, who included actual operational data in the modelling. However, if particulates were to be included, it is expected that the temperatures obtained would be lower.

Conclusions

The waste-heat boiler is the common choice for heat recovery and dust collection in pyrometallurgical processes. According to the literature it is clear that successful operation of the boiler requires sufficient understanding of the process and its operating conditions. Computational fluid dynamic modelling did prove to be a valuable aid in providing insight into the flow and temperature profiles within the waste-heat boiler. It was possible to identify and quantify the contribution of turbulence and radiation effects. However, most of the analysis was done qualitatively. Based on the findings obtained, the following significant conclusions can be made:

- The geometric modifications that were investigated revealed the elevation of the front radiation ceiling and the placement of a sunken baffle halfway within the radiation section to be very effective in cooling the hot off-gas more rapidly and increasing the residence time for dust segregation. This was the result of the off-gas stream being forced to follow an S-shaped flow path, which is considered much more effective than the straight gas stream along the straight roof of the conventional waste-heat boiler design.

- The effect of introducing circulated off-gas at the optimum angle of 45° and speed of 20 m/s was found to further enhance cooling while preventing a high impact on the boiler roof refractory.

- The placement of radiation plates did have the desired effect of further enhancing the heat transfer while also distributing the off-gas flow more evenly through the waste-heat boiler. The final recommended design includes the placement of a row of radiation plates (4 plates) after the inlet, a second row (8 plates) before the sunken baffle, a third row (8 plates) behind the sunken baffle and a tightly spaced last row (7 plates) prior to convection section.

- The off-gas SO₂ content must be maintained at an optimum of 45% since a higher composition will result in a high heat duty placed on the boiler refractory while lower compositions will allow cold areas to form, which in turn would lead to fouling.

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References