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THE DEVELOPMENT AND APPLICATION OF A CFD MODEL OF COPPER FLASH SMELTING

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ABSTRACT

A comprehensive CFD model has been developed of the direct to blister (DBF) copper flash smelting furnace at BHP Billiton's Olympic Dam facility. The model is based on commercial software (ANSYS-CFX) and uses the well-established Lagrangian particle tracking methodology to capture the important inter-phase transfer of heat, mass, and momentum. Lab-scale experimental data, taken from drop-tube tests, were used to develop a detailed sub-model that describes the very complex process of thermal decomposition and combustion that the copper concentrate particles undergo in flash smelting. A series of plant trials were undertaken to validate the model. The model has since been used to understand the sensitivity of the furnace performance to a range of operating parameters and mechanical modifications, providing valuable guidance for the furnace operation and maintenance. The model also played a key role in the development of an improved disperser (central-lance), which has yielded nearly a 10 percent increase in the furnace oxygen efficiency.

INTRODUCTION

In the flash furnace, shown schematically in Figure 1, sulphide concentrate, silica flux, pure oxygen, oxygen enriched air, and hydrocarbon fuel are introduced at the top of the reaction shaft. Concentrate particles are heated and undergo thermal decomposition and combustion which liberates sulphur and sulphur dioxide to the gas phase. In the gas phase the liberated sulphur combusts to sulphur dioxide. In flash smelting generally, the molten oxidised particles are collected in the settler where further reactions with the flux occur. In copper flash smelting a metal (blister-copper) or copper-iron-sulphur matte phase and a fayalite slag phase are formed and separated by gravitational settling. Slag and metal (or matte) are tapped from the furnace at regular intervals. Waste gases leave through an uptake shaft which continues to a waste heat boiler and electrostatic precipitator for heat and dust recovery.

The concept of an industrial processing route for copper and copper-nickel concentrates based on flash smelting was first suggested in 1936, but actual commercial development did not proceed for more than a decade (Habashi 1998). By the early 1950's both Inco (Copper Cliff, Canada) and Outokumpu (Harjavalta, Finland) were operating industrial scale flash smelters and flash smelting now delivers more than 50% of the world's primary copper production with more than 40 smelting facilities around the globe.

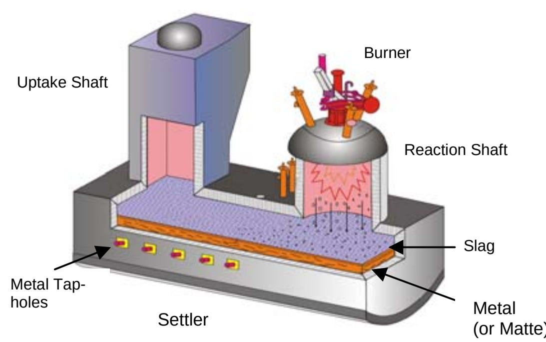

Figure 1: Schematic of flash smelting furnace.

The flash smelting process has long been a target for CFD modelling and published research can be found in the very first of the CSIRO series of conferences on CFD in the Minerals and Process Industries (Koh et al 1997, Ahokainen et al 1997). Šutalo et al (1998a,b) provided fundamental insight into the details of the fluid flow in the near-burner region of industrial flash smelters through detailed experimental and computational modelling. Since that time, in conjunction with the advances in commercial software, more sophisticated CFD models have been developed, both geometrically and phenomenologically, allowing full 3D treatments of actual commercial installations and improved sub-models of radiation heat transfer (Vaarno et al 2003, Ahokainen et al 2006) and particle behaviour (Solnordal et al 2003,2009). Unfortunately, physical measurements at full scale in support of CFD models are practically very difficult and only limited data have been published in this regard (Parada et al 2006, Jorgensen et al 2005). Many researchers have approached the issue of validating CFD models of flash smelting by modelling simpler laboratory scale systems such as laminar flow furnaces (i.e. drop-tubes) (Adams et al 1999, Hahn and Sohn 1990).

Drop-tube experiments (Jorgensen 1983, Peuraniemi and Jokilaakso 2000) have more generally provided insight into single particle behaviour including the pyrolysis and combustion of copper concentrates, and these and other similar studies, many of which feature in the review by Sohn and Chaubal 1993, are an important fundamental input to all CFD models of flash smelting. Unfortunately there is still much spread in the kinetic rate data, at least partially because of the difficulty of these experiments, but also because of the differences in the geology and chemistry of the many different concentrates.

In consideration of CFD models of the real flash furnace, further uncertainty is introduced due to the effects of particle break-up, particle-particle interactions such as agglomeration and other effects resulting from the high solids loadings that feature in industrial systems including, for example, "cloud" behaviour of dense solid suspensions (Caffrey 2002). Notwithstanding the remaining fundamental weaknesses in state-of-the art CFD models of flash smelting (Ahokainen et al 2006), model development (or improvement) is not the focus of the work reported here. It is instead the practical application of a CFD model to a real operating furnace that is of primary interest.

A reasonably comprehensive CFD model of a copper flash smelting furnace has been developed based on commercial CFD software, standard modelling techniques, and available literature. The specific focus is on the practical application of the model to the direct to blister furnace (DBF) of BHP Billiton at their Olympic Dam facility. The following chapters detail the model development and outline its use in the operation, maintenance and process improvement of the copper flash smelting furnace at Olympic Dam.

MODEL DESCRIPTION

Scope

As shown in Figure 2, the CFD modelled domain includes the disperser, reaction shaft, settler freeboard, and uptake shaft terminating effectively at the cross-over to the waste heat boiler.

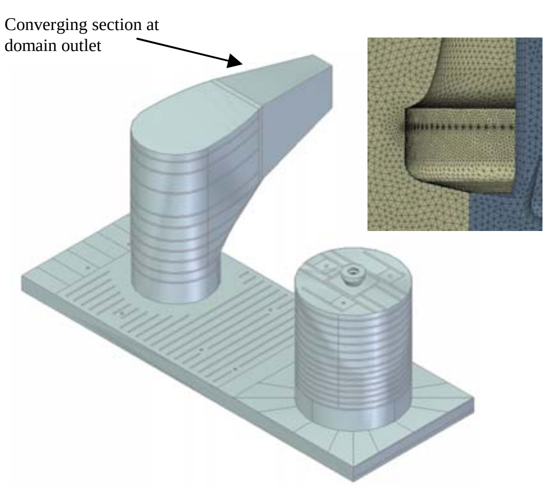

Figure 2: Geometry of CFD model of flash smelting furnace. Fine mesh on disperser shown top right.

For reference, the distance from the top of the reaction shaft to the slag surface is approximately 6 metres. To promote convergence in the computations, the domain outlet is formed with a small converging section to eliminate the tendency for recirculation in this region. The 3 roof-mounted oil burners are included. Thermal boundary conditions on the reaction shaft and settler walls accounted for water cooled elements by simply specifying an equivalent effective thermal resistance (including inner refractory, conduction through the copper cooler, and film resistance at the cooling passage/water interface) and a specified cooling water temperature. Heat loss through the non-water-cooled refractory wall was insignificant compared to the water-cooled elements and was ignored.
A full 3D treatment was used and the geometric details of the very small (4 and 5 mm diameter) gas inlets associated with the dispersion air were captured (shown Figure 2). The practical operation of the furnace is based on a specified enriched air velocity set-point which is achieved by the movement of the "velocity-cone device". This is fundamentally a geometric modification which adjusts the annular gap through which the enriched air must pass: the gas velocity is increased by lowering the velocity-cone thereby reducing the gap area. As a result, a partial re-meshing of the domain is required for each operating position of the velocity-cone. A cross section of the geometry through the burner and upper reaction shaft centre line is shown in Figure 3.

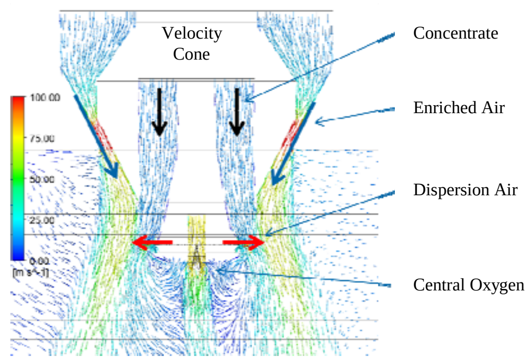

Figure 3: Cross section of burner and disperser.

Mesh

An unstructured mesh with triangular surface elements and tetrahedral volume elements was used throughout the domain. The complete mesh was comprised of 3,200,000 tetrahedral elements (700,000 nodes) using fine mesh near the disperser.

Mesh inflation at solid surfaces was used to capture the boundary layer effects on key solid surfaces including the disperser and reaction shaft walls. Mesh controls were used to produce a fine mesh (element size 0.01 m) with good resolution of the gas and solid behaviour within the main combustion plume just below the disperser. The mesh within the uptake and converging outlet portion of the domain were relatively coarse with representative element sizes of 0.2 m.

MODEL DEVELOPMENT AND VALIDATION

Essential Features

The computational model was based on the commercially available software package ANSYS-CFX v14 which uses a standard finite volume formulation of the "Reynolds Averaged Navier Stokes" (RANS) equations. Gas-phase turbulence was modelled following the Shear Stress Transport (SST) approach of Menter (1994). Lagrangian particle tracking of the injected solid-phase copper concentrate, flux, and dust using representative size fractions provided the framework for modelling the inter-phase transfer of mass, momentum and energy. Between 12,000 and 24,000 representative particles were "tracked" for each steady-state solution, with concentrate particle sizes of 25 and 35 microns and return dust and flux particle sizes of 194 and 169 microns respectively. The mineralisation of the two representative size concentrate particles was specified to reflect the particle size based mineral content variation that has been measured on site. The high solids loading and strong coupling between gas- and solid-phases required significant under-relaxation of the inter-phase transport rates. Gas-phase combustion (S_2 oxidation to SO_2) was modelled using the turbulence controlled (mixing limited) model of Magnussen and Hjertager (1976). A standard P-1 model was used for radiation heat transfer.

Kinetic Sub-Models

A total of 12 chemical reactions of importance were identified to describe the process of concentrate particle thermal decomposition and oxidation (Table 1). Arrhenius rate expressions, based on the particle temperature, were used to describe the (five) decomposition reactions (those liberating gaseous sulphur or oxygen). The (seven) oxidation reactions were modelled assuming that oxygen diffusion to the particle surface is also potentially rate determining.

	Type	Reaction Equation
A	Decomp.	$2CuFeS_2 = Cu_2S + 2FeS + 0.5S_2$
B	Decomp.	$2\ Cu_5FeS_4 = 5Cu_2S + 2\ FeS + 0.5S_2$
C	Oxidation	$Cu_2S + 1.5O_2 = Cu_2O + SO_2$
D	Oxidation	$Cu_2S + O_2 = 2Cu + SO_2$
E	Decomp.	$4CuS = 2Cu_2S + S_2$
F	Oxidation	$CuS + O_2 = Cu + SO_2$
G	Decomp.	$CuSO_4 = CuO + 0.5O_2 + SO_2$
H	Decomp.	$2\ FeS_2 = 2FeS + S_2$
I	Oxidation	$3FeS + 5O_2 = Fe_3O_4 + 3SO_2$
J	Oxidation	$FeS + 1.5O_2 = FeO + SO_2$
K	Oxidation	$3FeO + 0.5O_2 = Fe_3O_4$
L	Oxidation	$2\ Fe_3O_4 + 0.5\ O_2 = 3\ Fe_2O_3$

Table 1: Chemical reactions modelled to describe the concentrate particle thermal decomposition and oxidation.

Drop-tube Experiments

To test and validate the kinetic scheme, a simplified CFD model was used to reproduce the drop-tube experiments of Sohn and Chaubal (1993) simulating the combustion of chalcopyrite (70%) and pyrite (30%). The apparatus used for the experiments consisted of a drop-tube cylinder of 230mm diameter, 20mm diameter inlet, and 1.2m length. In addition, the experiments utilised:

- A high loading of particles, with 0.00133kg/s of concentrate feed and 0.001523kg/s of process gas.
- Process gas with an oxygen content of 21%.
- Solid particles, with a mass mean diameter of 47.3µm.
- An average particle density of 4300kg/m^3.
- Heated walls with controlled thermal conditions.

Some typical results (gas phase temperature contour and particle composition history) are shown in Figure 4.

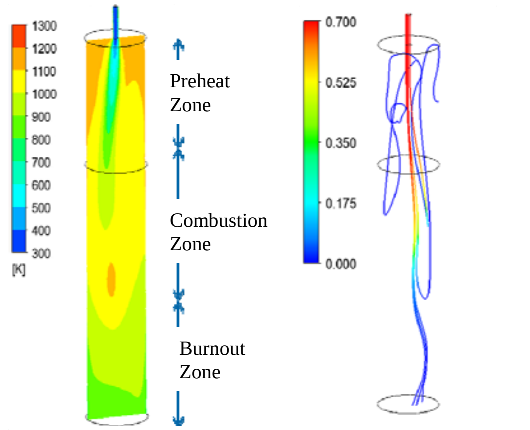

Figure 4: Qualitative CFD model results for drop-tube experiments.

As shown in Figure 5, the CFD model predicted the sulphur removal behaviour of particles in the drop-tube reasonably overall, but over-predicted the ignition delay time. The experimental measurements suggest that the reactions are initiated sooner than the model predicts.

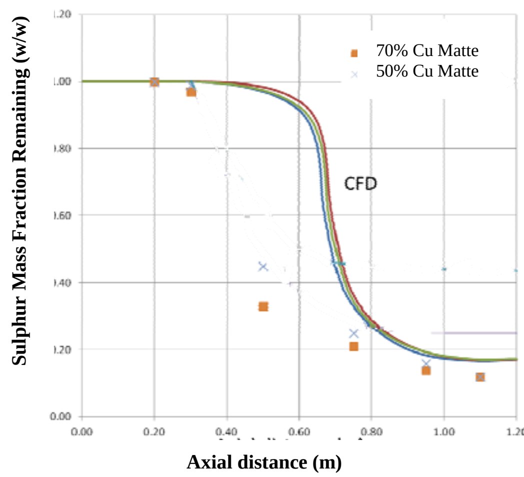

Figure 5: Comparison of CFD model results with experimental data of Sohn and Chaubal (1993).

Plant Trials

Data collected from plant trials at Olympic Dam and as recorded by the SCADA system were also used to validate the CFD model. The plant trials required furnace operation at steady conditions for a minimum of 12 hours to allow a steady state to be reached. Gas temperature measurements from different positions within the reaction shaft and oxygen concentration at the furnace outlet were collected.

Varying operating conditions were used for validation purposes including; different feed rates, enriched air velocities and Cu:S ratio of the feed. This last condition is effectively the change in the heat content (i.e. fuel sulphur) of the concentrate that results from the variation in ore grade.

Temperature Measurements in the Reaction Shaft

A novel method was devised to collect temperature profile data in the reaction shaft. This consisted of curved mild steel box section probes wrapped in unifrax insulation with K-type thermocouples at various positions along their length and an R-type thermocouple at the end of the probe.

Four radiused probes and a single straight probe were constructed which allowed measurements at different points in a plane approximately at mid-elevation of the reaction shaft (3.5 meters above the settler roof and 2.3 meters below the reaction shaft roof). This technique allowed simultaneous multi point measurements across the entire reaction shaft with nine probe insertions. Figure 6 shows a probe in the process of being retracted from the reaction shaft.

Figure 6: Probe being retracted from reaction shaft.

Figure 7 shows the measured temperature profile at the sampling plane for a single measurement set and the curved probes used to take the measurements. It is worth noting that when the probes were removed from the furnace, concentrate deposited on the probe continued to react and release SO_2.

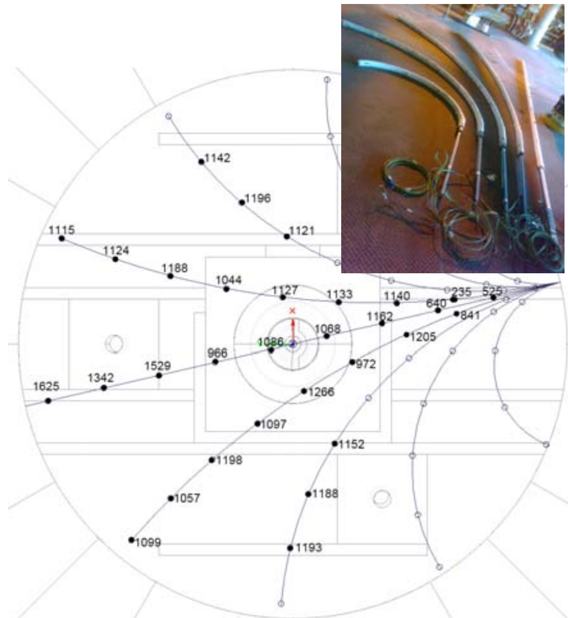

Figure 7: Gas-phase temperatures (^{o}C) measured at site with Case 3 (refer Table 2) operating conditions. Measurement probes are shown in top right.

	Feed Rate (tph)	Cu:S	Gas Enrich. (O_2 %)	Enrich. Air Velocity (m/s)	Mom. Ratio (%)	Disperser hole (mm)
1	50	1.77	60	95	25	4
1A	50	1.77	60	95	25	4
2	60	1.73	60	100	25	4
3	50	1.67	66	100	25	4
4	60	1.73	60	100	16	4
4A	60	1.73	60	100	30	5
5	60	1.73	60	100	25	(Swirl)
6	60	1.73	60	100 (17^{o})	25	4
6A	60	1.73	60	100 (45^{o})	25	4
6B	60	1.73	60	100	25	4
7	70	1.30	50	60	23	4
8	70	1.30	50	100	23	5
9	70	1.30	60	100	23	5
10	60	1.73	60	100	25	4

Table 2 Key furnace operating parameters for the cases examined.

APPLICATIONS OF THE MODEL

Validation and Production Cases

The key parameters for the complete set of simulation cases that were undertaken are provided in Table 2. Cases 1, 1A, 2, and 3 used inputs the same as those prevailing during the sampling periods for the plant trial. The objective of these runs was to tune and validate the complete CFD model. Identical inputs were used for Cases 1 and 1A, with the latter using a non-ideal concentrate feed distribution that was computed using a discrete element model (DEM) and used as input into the CFD.

Cases 4, 4A, 5, 6, 6A, and 6B used a wider range of inputs and changes to the system geometry with the objective of developing a mechanical configuration with improved smelting performance by understanding the sensitivity of the smelting process to the specific details of the disperser and burner assembly. Case 5 assessed the effect of swirling of the dispersion air, and cases 6 and 6A swirling of the enriched air at angles of 17 and 45 degrees, respectively. Case 6B examined the effect of a shaped disperser head that would provide better distribution of concentrate directly below the disperser. Cases 7, 8, and 9 focussed on smelter performance when operating with lower feed grades to optimise the furnace performance under such conditions.

Finally, case 10 investigated the effects of misalignment of the burner block within the reaction shaft to assist plant personnel in establishing maintenance priorities.

Velocity and Temperature Profiles

The velocity vector plot at the centre plane of the reaction shaft and the overall flow regime are shown in Figure 8. The results are consistent with other 3D models of industrial scale flash smelters (Solnordal 2003, 2009), showing the expected strong downward central jet with local recirculation below the disperser head and a strong overall circulation upwards at the reaction shaft walls.

The system is asymmetric because of the major flow path from reaction shaft along the settler to the uptake. This gives rise to a stronger recirculation (and higher temperatures) along the reaction shaft wall furthest from the uptake (see Figure 8 and Figure 9). Within the combustion plume, directly below the disperser, is a colder core region. This is also consistent with other CFD models and characteristic of most diffusion flames in industrial applications.

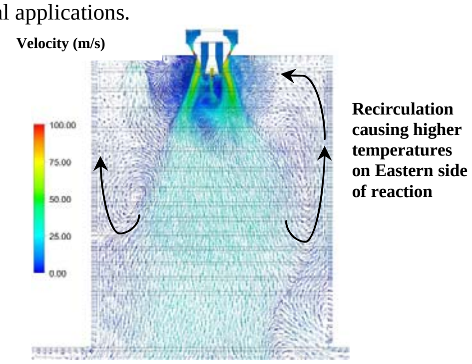

Figure 8: Gas velocity vectors at centre-plane of reaction shaft (Case 2).

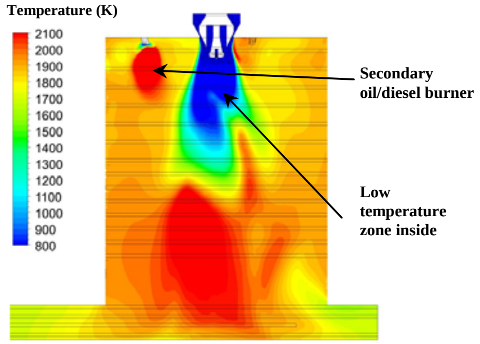

Figure 9: Gas-phase temperature contour at centre-plane of reaction shaft (Case 2).

Comparison of computed and measured temperatures along the single straight insertion probe is given in Figure 10. Thermocouple measurements are generally higher than CFD predictions for this dataset (Case 3). During insertion it was noted that the probes were coated with molten concentrate particles. It was thought that the coated thermocouples were producing a more uniform temperature distribution. Low temperature measurements at the extremity of the reaction shaft were also observed. A possible cause for this behaviour is furnace ingress air cooling the thermocouple through the furnace port.

Both drop-tube and plant measurements suggested that the CFD model was under-predicting the rate of particle heating so the particle emissivities were increased to 0.80. No further changes were made to tune the CFD model and the same model parameters (chemistry and heat transfer) were used for all simulations.

Incidental values such as exit temperatures matched trends predicted by the different CFD runs. In addition, observations of gas flow in the furnace also matched CFD results. For example, observations of upward moving gas at the reaction shaft walls were consistent with the recirculation zones seen in the CFD model.

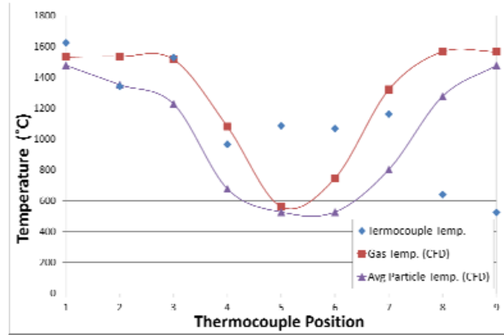

Figure 10: Comparison between site measurement and computed reaction shaft centreline temperature (Case 3).

Heat Loss from Reaction Shaft

The reaction shaft of the furnace is constructed of water-cooled copper elements. The heat load from each element is measured continuously and this was used to compare with the heat loss on comparable sections of the CFD model.

A comparison of actual and predicted heat loss for the upper, middle, and lower portions of the reaction shaft wall is given in Table 3. The average error is between 1 and 32 percent for the reaction shaft elements and 59% for the transition elements at the bottom of the reaction shaft connecting to the settler. While the agreement is not particularly good, it must be noted that the heat loss from these elements will depend strongly on the presence of accretions on (or loss of refractory from) the furnace walls, which the CFD model does not take into account. Wall accretions will act in an insulating capacity and reduce the heat loss from the reaction shaft. Conversely, where refractory brick and/or the water-cooled copper elements have been worn, the actual heat loss can be significantly greater than predicted.

Location	**Predicted** (MJ/h)	**Measured** (MJ/h)	**Error** (%)
Upper	2436	3577	32
Middle	2037	2416	16
Lower	2159	2182	1
Transition	1872	4535	59

Table 3: Reaction shaft heat loss (Case 2)**.**

Gas Species

Oxygen concentration of the furnace off-gas was monitored over a 16 hour period. Data from this investigation determined that the actual oxygen composition varied from 2 to 4 wt%. The CFD model predicted approximately 5 wt% oxygen concentration in off-gas at the reaction shaft outlet (Figure 11) which was also comparable to measurements.

Sulphur dioxide produced from the exothermic multiphase reactions was examined for all cases. High concentrations of SO_2 were observed in the middle and lower portion of the reaction shaft. Transport of SO_2 from the strong recirculation behaviour was also seen (Figure 12).

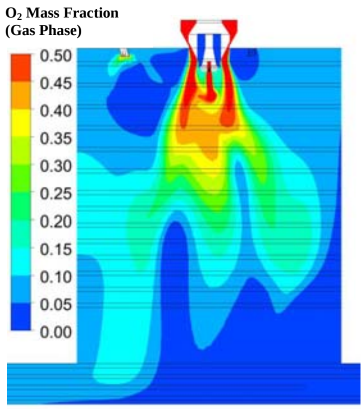

Figure 11: Typical computed oxygen mass fraction at centre plane of furnace (case 2).

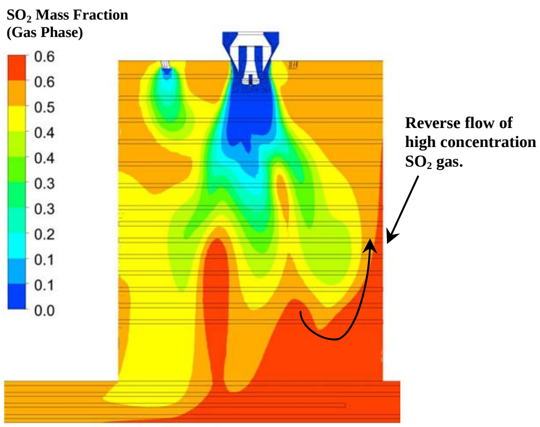

Figure 12: Typical computed SO_2 mass fraction at centre plane of furnace (Case 2).

Model Application

The combustion performance of the Olympic Dam DBF can be expressed in terms of the sulphur removed from the concentrate as a function of vertical distance below the injection point (Figure 13). Evaluations of the cases listed in Table 2 were used to investigate the benefits of potential changes to mechanical configuration (Cases 4-6B) and to evaluate appropriate process responses to change in feed grade (Cases 7-9).

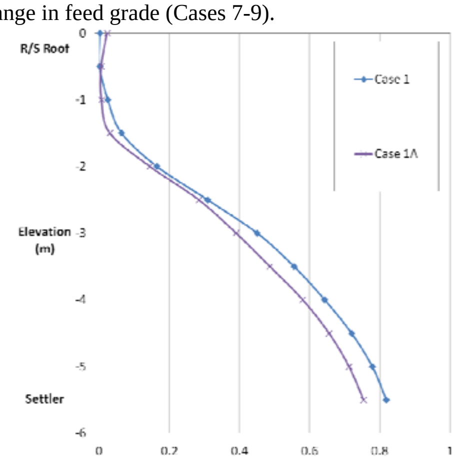

Figure 13: Typical sulphur removal behaviour.

DEVELOPMENT OF A NEW DISPERSER

Concept and Implementation

Of considerable significance, a comparison of the CFD analysis from Cases 1 and 1A (Figure 13) established the importance of a uniform solid feed to the flash smelter. With an ideal mass flow of solids (i.e. both radial and circumferential uniformity), there is nearly a 7% improvement in predicted sulphur removal. To this end a new disperser design was developed that provided a concentrate distribution that was nearly ideal (maximum variation circumferentially of less than 5% of the mean solids mass flow rate). The full-scale prototype of the new disperser is shown in Figure 14. Subsequent study has continued to investigate the importance of both spatial and temporal uniformity in the delivery of the concentrate to the burner (Kokourine et al 2015).

Figure 14: New disperser prototype prior to installation in Furnace.

Results

When installed in the Olympic Dam flash smelter during its initial trial Sept 2014 the new disperser provided a dramatic improvement in the performance of the furnace. Oxygen in off-gas dropped significantly (Figure 15) and the calculated oxygen efficiency of the furnace increased by nearly 10 percent. Operators were able to achieve the same slag and metal chemistry while consuming significantly less oxygen in the enriched air stream. The smelter was able to maintain stable combustion without the need for roof-mounted auxiliary fuel burners. The reduction in oxygen consumption (compensating for the increased efficiency) meant that heat loads on the reaction shaft roof and sidewalls were unchanged from the original operation.

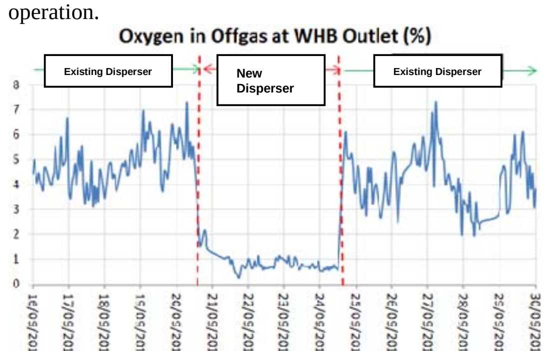

Figure 15: Oxygen content in off-gas during trial of new disperser.

SUMMARY AND CONCLUSIONS

The CFD model described in this paper has contributed to the understanding of gas dynamics and combustion in the flash smelting furnace at Olympic Dam. While predictions of exact temperatures, compositions or flows were not the motivation for the model development, confidence in the predicted results has been obtained. The

CFD model has provided a fundamental understanding of the furnace and delivered a powerful tool that can assist in evaluating furnace process improvements. To date the CFD model has already contributed to the development of a new disperser with significantly improved combustion performance. The success of the improved disperser demonstrates the power of these modelling techniques and the very real value they can bring to an operating plant.

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