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SIMULATING AGGLOMERATION OF MOLTEN PARTICLES IN THE FLASH SMELTING REACTION SHAFT

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ABSTRACT

A numerical model is developed to investigate the agglomeration of molten particles in the reaction shaft of a flash smelting process. In addition to simulating the turbulent, particle-laden, gas flow from the burner into the reaction shaft, a population balance model is incorporated to evaluate the agglomeration of particles as they collide and combine. It was found that the inlet particle volume fraction, the inlet mono-dispersed particle size, and the inlet turbulence intensity influence particle agglomeration in such a way that they could potentially be used to control and reduce dust losses. The angle of inflow from the burner into the reaction shaft was also found to influence predictions, with an abrupt change in behaviour identified to occur above a critical value that requires further examination. Predictions are found to compare well to related experimental data and numerical results found in the literature.

NOMENCLATURE

A	area (m^2)
c	collision rate expression (m^{-3} s^{-1})
d	particle diameter (m)
I	turbulent intensity (-)
k	turbulent kinetic energy (m^2/s^2)
N	particle number density (m^{-3})
r	radial distance from central axis (m)
u	radial velocity component (m/s)
$\mathbf{u}$	velocity vector (m/s)
v	particle volume (m^3)
w	vertical velocity component (m/s)
z	vertical distance from inlet (m)
δ	interpolative function (-)
η	interpolative function (-)
μ	moment of a distribution
ν	kinematic viscosity (m^2/s)
θ	inflow angle (degrees)
ρ	density (kg/m^3)
σ	Prandtl number (-)
ψ	volume fraction (-)

Subscripts:

avg	average
c	critical
d	drift
g	gas phase
i	particle phase number (or *p* for overall particle phase)
in	inlet
m	mixture
out	outlet
T	turbulent
1	mono-dispersed (i=1)

INTRODUCTION

The flash smelting process is used around the world in the production of copper from its sulphide ores. Concentrate particles are injected through a burner into a high temperature reaction shaft where they heat, ignite and react with oxygen-enriched air to produce molten slag and copper-rich matte/blister phases. A waste gas stream is also produced which is removed from the furnace via a separate offtake shaft.

Dust losses from the process occur when small particles become entrained in the waste gas stream. This reduces product recovery and additional maintenance is required to deal with accretion build-ups in and beyond the offtake shaft. Moreover, the dust needs to be removed from the waste gas stream to allow the effective production of sulphuric acid. Dust losses are typically 5-10wt% of the feed and feature particles of diameters up to around 100μm.

Themelis et al. (1988) developed a one-dimensional numerical model of the flash smelting reaction shaft which predicted the agglomeration of particles that were fed as molten. Unfortunately few details about the model were mentioned and only one set of predicted results were presented. Nevertheless the predicted evolution in the average particle diameter was significant and compared well with experimental data. The potential for using agglomeration to reduce dust losses was identified with the recommendation for further research on agglomeration in the process. However, since then, no further work focused on investigating or understanding the formation of agglomerates within the flash smelting process has been carried out (Donizak et al., 2005).

This work examines agglomeration in the flash smelting process by developing a numerical model of the reaction shaft that improves on the attempt of Themelis et al. (1988). This model is used to identify important process variables that influence agglomeration.

MODEL DESCRIPTION

Model Equations

The constitutive equations of the Algebraic Slip Mixture Model (Manninen et al., 1996) in conjunction with the two-equation k-ε model of Launder and Spalding (1974) are used to predict the turbulent, particle-laden, gas flow within the reaction shaft. The particle phase is partitioned into a set of separate phases according to the discrete population balance (DPB) of Kumar and Ramkrishna

(1996), where each particle phase *i* is made up of spherical particles of a specific volume v_i, and $v_i=2v_{i-1}$.

Here binary particle-particle interactions are assumed to be the dominant method by which particles agglomerate, which involves first the collision between a pair of particles followed by their combination into a single larger particle (i.e. $v_i=v_j+v_k$). The following collision rate expression is employed to predict the frequency of collisions between two particles of volumes v_i and v_j due to relative motions generated by turbulent mixing and phase slip (Nijdam et al., 2006),

$$c_{i,j} = \frac{\pi}{4}\left(d_i^2 + d_j^2\right)N_i N_j \sqrt{\left|\mathbf{u}_i - \mathbf{u}_j\right|^2 + 4k_m} \qquad (1)$$

where d_i, N_i and $\mathbf{u}_i$ are the particle diameter, particle number density and velocity vector of particle phase *i*, respectively, k_m is the mixture turbulent kinetic energy, and $c_{i,j}$ is the collision rate between particles of phases *i* and *j*. This expression was developed and validated for similar flow conditions and particle sizes to those considered here.

In accordance with the experimental findings of Kemori et al. (1988) and Kimura et al. (1986), colliding particles are assumed to combine together if they are in a molten sticky state. Themelis et al. (1988) assumed the particles were fed as molten. By predicting the heating and melting of particles that are fed as solid, it is found that the particles rapidly become molten after entering the reaction shaft such that differences in agglomeration behaviour when compared to predictions where the particles are assumed to be fed as molten are negligible (Higgins and co-workers, 2008, 2009). Consequently, the particles are assumed be fed as molten.

The fixed-pivot method (FPM) DPB (Kumar and Ramkrishna, 1996) is used to account for the effects on the particle size distribution (PSD) of agglomeration between pairs of particles. The continuity transport equation for each particle phase *i* is expressed as,

$$\nabla\cdot\left(N_i\mathbf{u}_m\right) = \nabla\cdot\frac{\nu_{m,T}}{\sigma_i}\nabla N_i - \nabla\cdot\left(N_i\mathbf{u}_{d,i}\right) + S_{A,B}\left(v_i\right) - S_{A,D}\left(v_i\right) \qquad (2)$$

where $\nu_{m,T}$ is the turbulent kinematic viscosity of the mixture phase, and σ_i is the Prandtl number of phase *i* (set as unity), $\mathbf{u}_m$ and $\mathbf{u}_{d,i}$ are the vectors of the mixture phase velocity and the drift velocity of particle phase *i*, respectively, where $\mathbf{u}_i=\mathbf{u}_m+\mathbf{u}_{d,i}$ (Manninen et al., 1996). The source terms of $S_{A,B}(v_i)$ and $S_{A,D}(v_i)$ evaluate the birth and death rate of particles of phase *i* (of particle volume v_i) due to agglomeration, respectively,

$$S_{A,B}\left(v_i\right) = \sum_{\substack{j,k \\ v_{i-1}\le v \\ v\le v_{i+1} \\ v=v_j+v_k}}^{j\ge k}\left(1-\tfrac{1}{2}\delta_{j,k}\right)\eta c_{j,k} \qquad (3)$$

$$S_{A,D}\left(v_i\right) = \sum_{k=1}^{M} c_{i,k} \qquad (4)$$

with,

$$\delta_{j,k} = \begin{cases} 1 & j=k \\ 0 & otherwise \end{cases} \qquad (5)$$

$$\eta = \begin{cases} \left(v_{i+1}-v\right)/\left(v_{i+1}-v_i\right) & v_i \le v \le v_{i+1} \\ \left(v-v_{i-1}\right)/\left(v_i-v_{i-1}\right) & v_{i-1} \le v \le v_i \end{cases} \qquad (6)$$

where *M* is the total number of particle phases (set as 25), v_{i-1} and v_{i+1} are the volumes of particles in phases that are adjacently smaller and larger to particle phase *i*, respectively, $\delta_{j,k}$ and η are terms used to conserve both total number and volume of particles (Kumar and Ramkrishna, 1996).

Numerical Considerations

The flow geometry of the burner and reaction shaft in which the occurrence of agglomeration is investigated is simplified to that of a sudden expansion, with the inlet diameter set as 1m and the outlet diameter and height both set to 5m (see Figure 1). The system is assumed to behave in a steady-state and axi-symmetric manner, though its behaviour is more likely both transient and three-dimensional (Sutalo et al., 1998). The numerical model is solved by a finite volume method using the commercial package Physica v2.12 (Cross et al., 1996). The two-dimensional, axi-symmetric plane of the simplified reaction shaft flow geometry is divided up into a uniform grid with side lengths of 0.1m. Source terms were discretised using central differencing and linearised where possible. The QUICK differencing scheme (Versteeg and Malalasekera, 1995) was employed elsewhere to evaluate advection terms, except for those in the mixture continuity and momentum transport equations where the power law scheme was used. Single phase flow predictions were used as starting conditions for all two phase cases solved. Sensitivity tests showed a variation of 5% in the predicted flow and transport profile results when the grid size was halved.

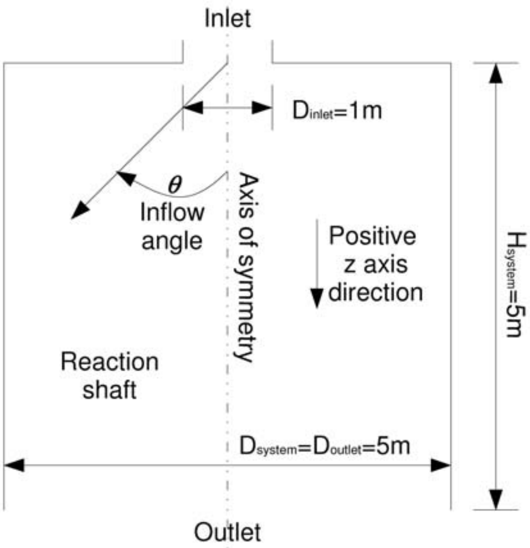

Figure 1: Schematic of flow geometry considered.

Inlet and Boundary Conditions

The PSD is set as mono-dispersed at the inlet to give a simple basis for evaluating the extent of agglomeration. Constant and uniform values for the: inlet vertical mixture velocity ($w_{m,in}$), angle of injected flow from inlet ($\theta = artan(u_{m,in}/w_{m,in})$, where u_m is the inlet radial mixture velocity), inlet particle volume fraction (in terms of $\psi_{p,in}=\psi_{i=1,in}$), inlet mono-dispersed particle diameter ($d_{p,in}=d_{i=1,in}$), inlet turbulence intensity ($I_{m,in}$) are specified at the burner boundary and used to evaluate other required

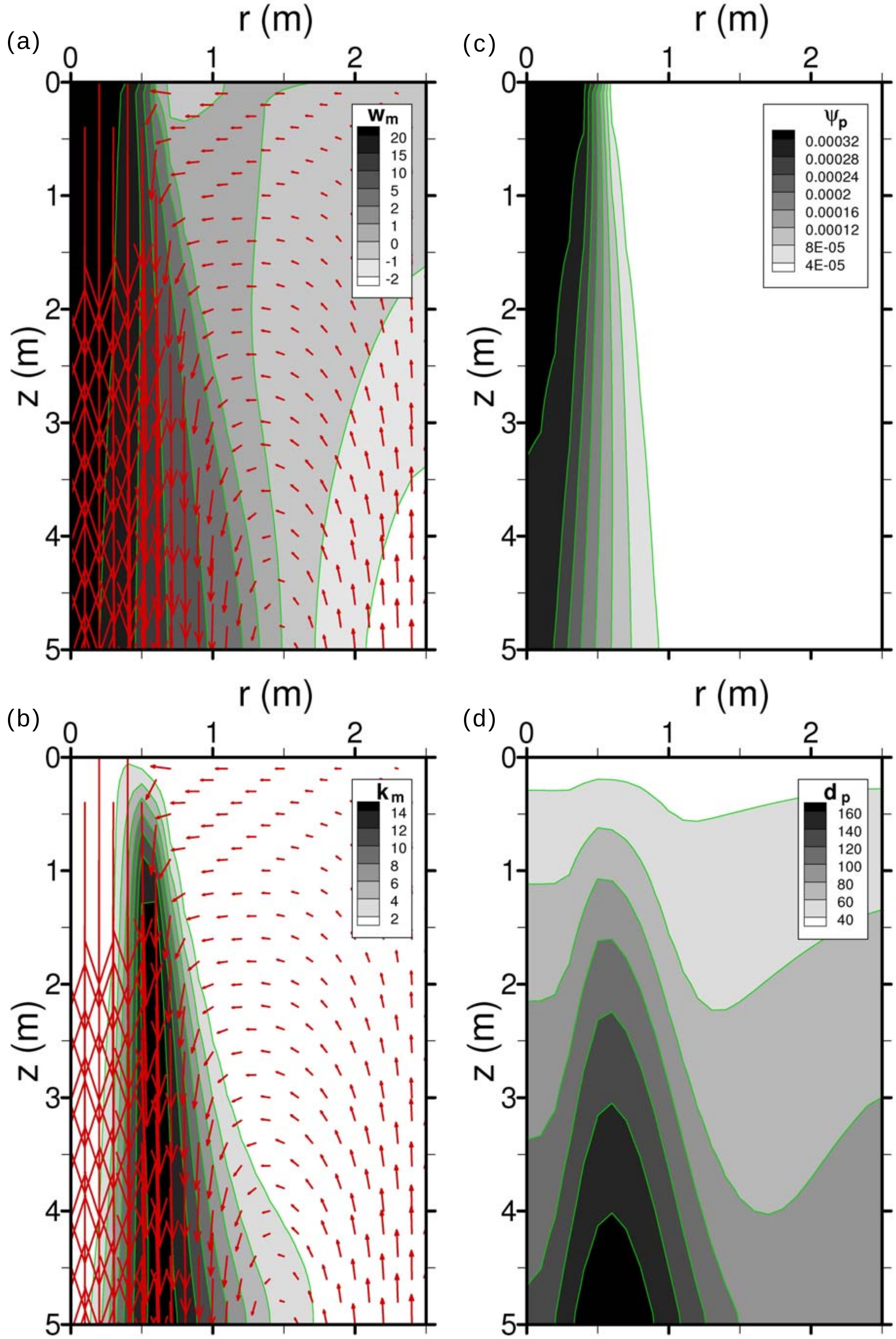

Figure 2: Contour plots of (a) vertical mixture velocity, w_m (m/s), with vector map, (b) turbulent kinetic energy, k_m (m^2/s^2), with vector map, (c) particle volume fraction, ψ_p, and (d) average particle diameter, d_{avg} (μm) for the case solved using the standard inlet variable values listed in Table 1.

inlet conditions such as $k_{m,in}$ and $N_{i,in}$. Zero flux conditions are specified at the walls and the standard log-law wall function is used to evaluate turbulence values in the elements adjacent to the walls (Versteeg and Malalasekera, 1995). The outlet is specified to have a zero gradient flux and a constant, uniform pressure. Phase properties are assumed to be constant and independent of conditions with ρ_p=3000 kg/m^3, ρ_g=1 kg/m^3, $\nu_g=2\times10^{-5}$ m^2/s.

RESULTS

To establish the flow and agglomeration behaviour predicted by the numerical model described above, a standard case is solved for the industrially relevant inlet variable values listed in Table 1. Figure 2 shows contour plots and vector maps of the standard case predictions. Figure 2(a) indicates the presence of a narrow, but intense, jet-flow region down the central axis region with a large, but weaker, recirculation zone adjacent to the walls. Figure 2(b) shows that these two regions are joined by a turbulent shear layer. In Figure 2(c) the majority of particles are found to travel down the jet-flow region and to be gradually dispersed into the recirculation zone by the turbulent shear layer.

Quantity	Value		
	Low (L)	Standard (Std)	High (H)
$w_{m,in}$ (m/s)	10	20	40
$I_{m,in}$	0.037	0.050	0.100
$\psi_{1,in}$	1.67×10^{-4}	3.33×10^{-4}	6.67×10^{-4}
$d_{1,in}$ (μm)	10	30	50
θ (degrees)		0	up to 60

Table 1: Modelling conditions.

Three quantities are evaluated to quantify the predicted agglomeration behaviour.

The first is the average particle diameter, d_{avg}, which is calculated (assuming the particles are spherical) by dividing the first PSD moment, μ_1 (total volume of particles), by the zeroth PSD moment, μ_0 (total number of particles), as follows,

$$\frac{\mu_1}{\mu_0} = \sum_i^M v_i N_i \Bigg/ \sum_i^M N_i = \frac{\pi}{6} d_{avg}^3 \qquad (7)$$

Secondly, to account for the effects of flow in and out of the system, the outlet average particle diameter, $d_{avg,out}$, is calculated as,

$$\frac{\mu_{1,out}}{\mu_{0,out}} = \frac{\pi}{6} d_{avg,out}^3 \qquad (8)$$

where $\mu_{0,out}$ and $\mu_{1,out}$ are akin to μ_0 and μ_1 only also evaluated as a function of the flow at the outlet of area A_{out} as,

$$\mu_{k,out} = \sum_i^M \int_0^{A_{out}} v_i^k N_{i,out} w_{i,out} dA_{out} \qquad (9)$$

Thirdly, $\Delta d_{out}\%$, denoted as the percentage change in the outlet average particle diameter, is calculated as,

$$\Delta d_{out}\% = \frac{d_{avg,out} - d_{avg,in}}{d_{avg,in}} \times 100\% \qquad (10)$$

where for a mono-dispersed inlet PSD $d_{avg,in}=d_{p,in}=d_{1,in}$. Figure 2(d) shows the contour plot of d_{avg} for the standard case with the rate of agglomeration and subsequent increase in d_{avg} being most significant in the shear layer (i.e. r~0.5m). For the standard case, $d_{avg,out}$=170μm and $\Delta d_{out}\%$=460%, which compares well with the experimental findings of Kemori et al. (1988) and Kimura et al. (1986), and the numerical results of Themelis et al.

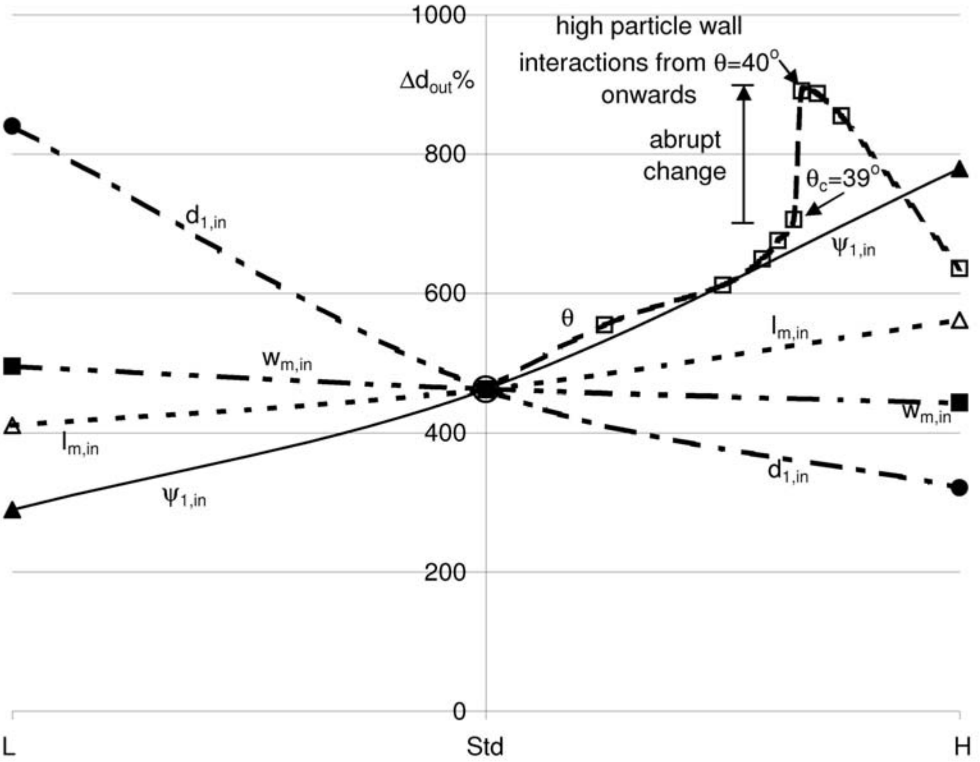

Figure 3: Values of the percentage change in the outlet average particle diameter, $\Delta d_{out}\%$, for individual variations in the indicated variables with all other variables fixed at the standard values. The variable magnitudes of L (low), Std (standard), and H (high) correspond to the labelling used in Table 1.

Parametric Study

To examine the effects of different variables on agglomeration, a series of cases are solved where the variables are individually varied to the non-standard, extreme values typically encountered in practice as listed in Table 1. With the predicted flow behaviour remaining largely unchanged from the standard case, Figure 3 showing the variation in agglomeration behaviour in terms of $\Delta d_{out}\%$ summarises the parametric study findings.

From Figure 3 it is found that variations in the inlet particle volume fraction ($\psi_{1,in}$) and inlet mono-dispersed particle diameter ($d_{1,in}$) influence $\Delta d_{out}\%$ the most significantly. These variables influence the inlet particle number density ($N_{1,in}$), and therefore the local particle number density, which appears twice as a proportional factor in the collision rate expression of Equation (1). $N_{1,in}$ is directly proportional to $\psi_{1,in}$ and inversely proportional to $d_{1,in}$ according to the relationship,

$$\psi_i = v_i N_i \qquad (11)$$

As a consequence, increasing $\psi_{1,in}$ and decreasing $d_{1,in}$ will cause $N_{1,in}$, the collision rate, and the extent of agglomeration to increase as predicted in Figure 3. Note that the influence of θ is also significant, and its trend is discussed in the next section.

Of the remaining two variables presented in Figure 3, $w_{m,in}$ has negligible influence on $\Delta d_{out}\%$, while the influence of $I_{m,in}$ is to have a proportional effect on $\Delta d_{out}\%$. Increasing both of these variables increases the level of turbulence at the inlet and therefore the local turbulence levels, i.e. k_m, which is also a prominent variable in the collision rate expression of Equation (1). However, increasing $w_{m,in}$ also decreases the average flow residence time, which seems to have the effect of cancelling out any gains in agglomeration from the additional turbulent mixing.

Inflow Angle

Figure 3 shows that the effect on $\Delta d_{out}\%$ of varying the inflow angle, θ, is both significant and unusual. Initially $\Delta d_{out}\%$ increases with θ, but after a critical value, i.e θ_c=39°, $\Delta d_{out}\%$ increases abruptly and then decreases with further increases in θ. Figure 4 shows the flow behaviour for (a) $\theta=\theta_c$=39° and (b) θ=40°. The predictions in Figure 4(a) are found to be similar to those in Figure 2(a) with an additional small recirculation zone below the inlet, while the predictions in Figure 4(b) are completely different with the flow direction of the main recirculation zone having switched.

The behaviour in Figure 4 explains the agglomeration trend predicted in Figure 3 for θ. With the gradual growth of the small recirculation zone below the inlet for θ values up to θ_c, agglomeration increases as the particle residence time increases. Then when the abrupt change in the flow behaviour occurs for $\theta > \theta_c$, the particle residence time increases significantly, and so does agglomeration, as the particles first travel towards the walls before leaving the shaft. As θ further increases, agglomeration decreases as the particle stream becomes more horizontal and the particles begin to fall out of the shaft closer to the inlet.

Reasons for this abrupt change in behaviour are unclear. Based on the work of Guo et al. (2001a,b) and Sutalo et al. (1998a,b) it is speculated that the predictions for the approximately similar θ inlet conditions of 39° and 40° may be indicative of transient, three-dimensional precession. However, investigation of this is beyond the capabilities of the presently developed steady-state, axi-symmetric model.

From a reducing dust losses point of view, the predictions in Figure 3 show that it would be beneficial to promote the spread of the flow radially outwards from the burner somehow, i.e. increase θ. However, when considering the

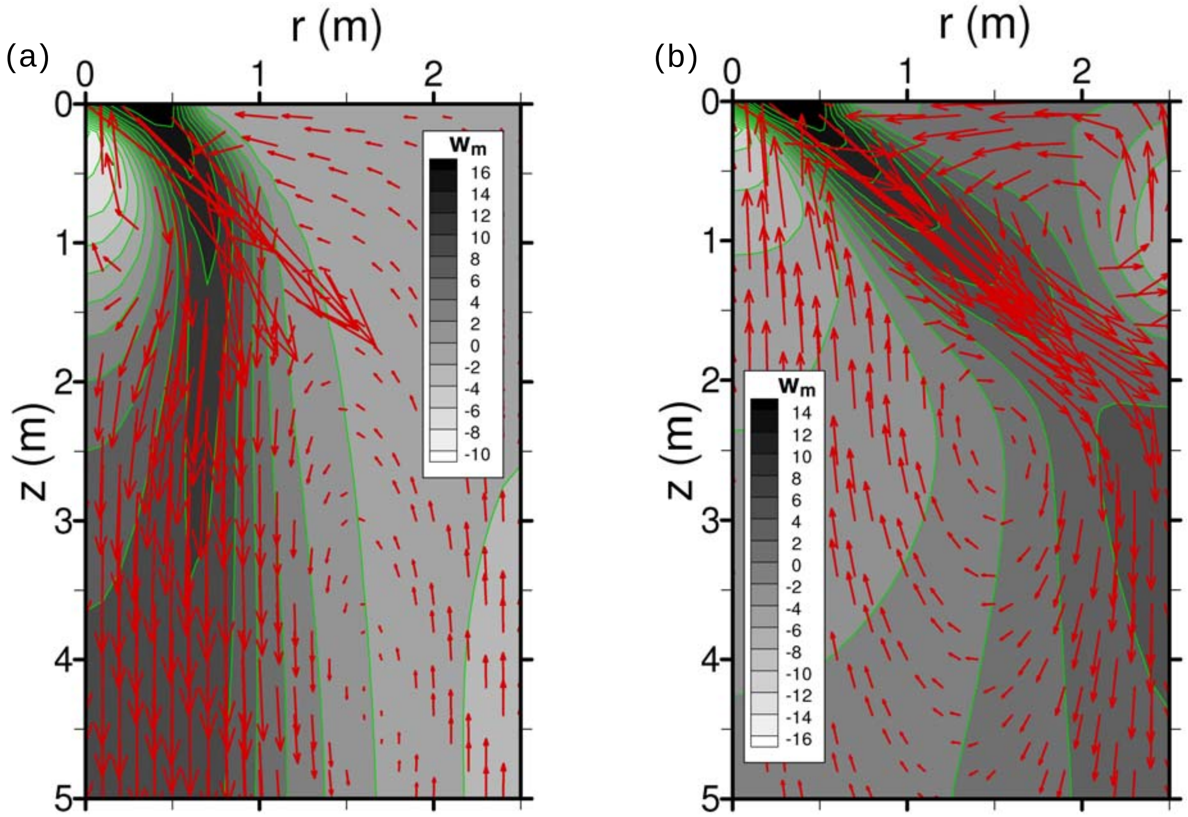

Figure 4: Contour plots of the vertical mixture velocity, w_m (m/s), with vector map, for two cases solved under the same standard conditions but with different θ values of (a) 39° and (b) 40°.

predictions in Figure 3 in combination with those in Figure 4 it is suggested that high θ values above θ_c be avoided as this would promote particle-wall interactions. The occurrence of particle-wall interactions is undesirable as it leads to increased maintenance requirements and increased operating costs due to refractory wear and accretion build-ups. Consequently, based on the findings presented above it would be best to operate at θ values up to θ_c=39°.

CONCLUSION

A steady-state, axi-symmetric, numerical model of the turbulent, particle-laden, gas flow for a flash smelting reaction shaft that predicts agglomeration behaviour in close comparison to published experimental and numerical results has been developed. The model was used to predict the effects of various variables on agglomeration with the variables of inlet particle volume fraction ($\psi_{1,in}$), inlet particle diameter ($d_{1,in}$), inlet turbulence intensity ($I_{m,in}$), and inflow angle (θ) identified as important. For the purposes of promoting agglomeration to reduce dust losses it is recommended best to adjust these variables so as to increase particle number densities (high $\theta_{1,in}$ and low $d_{1,in}$), turbulence levels (high $I_{m,in}$), and average flow residence times (high θ up to θ_c=39°). An abrupt change in behaviour is predicted for $\theta > \theta_c$ that needs to be further investigated using a transient, three-dimensional model.

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REFERENCES

CROSS M., CHOW P., BAILEY C., CROFT T.N., Ewer J., LEGGETT P., McMANUS K., PERICLEOUS K. and PATEL M.K., (1996), “PHYSICA – A Software Environment for the Modelling of Multi-Physics Phenomena”, *Z. Angew. Math. Mech. ZAMM*, **76**(S4), 105-108.

DONIZAK J., HOLDA A. and KOLENDA Z., (2005), “On the Evolution of Mathematical Modelling of Single-Step Flash Smelting of Copper Concentrates”, *Progress in Computational Fluid Dynamics*, **5**(3-5), 207-221.

GUO B., LANGRISH T.A.G. and FLETCHER D.F., (2001a), “Simulation of Turbulent Swirl Flow in an Axisymmetric Sudden Expansion”, *AIAA Journal*, **39**(1), 6-102.

GUO B., LANGRISH T.A.G. and FLETCHER D.F., (2001b), “Numerical Simulation of Unsteady Turbulent Flow in Axisymmetric Sudden Expansions”, *Journal of Fluids Engineering*, **123**(3), 574-587.

HIGGINS D.R., (2008), “Simulating Agglomeration in the Flash Smelting Reaction Shaft to Reduce Dust Production”, *Phd Thesis*, The University of Melbourne.

HIGGINS D.R., GRAY N.B. and DAVIDSON M.R., (2009), “Simulating Particle Agglomeration in the Flash Smelting Reaction Shaft”, *Minerals Engineering*, **22**(14), 1251-1265.

KEMORI N., OJIMA Y. and KONDO Y., (1988), “Variation of the Composition and Size of Copper Concentrate Particles in the Reaction Shaft”, *Flash Reaction Processes: Center for Pyrometallurgy Conf.*, University of Utah, Salt Lake City, Utah, June 47-68.

KIMURA T., OJIMA Y., MORI Y. and ISHII Y., (1986), “Reaction Mechanism in a Flash Smelting Reaction Shaft”, *The Reinhardt Schuhmann Int. Symp. On Innovative Technology and Reactor Design in Extraction Metallurgy*, AIME-TMS, Colorado Springs, Colorado, 403-418.

KUMAR S. and RAMKRISHNA D., (1996), “On the Solution of Population Balance Equations by Discretization – I. A Fixed Pivot Technique”, *Chem. Eng. Sci.*, **51**, 1311-1332.

LAUNDER B.E. and SPALDING D.B., (1974), “The Numerical Computation of Turbulent Flows”, *Comput. Methods Appl. Mech. Eng.*, **3,** 269-289.

MANNINEN M., TAIVASSALO V. and KALLIO S., (1996), “On the Mixture Model for Multiphase Flow”, *VTT Publications 288*, Technical Research Center of Finland.

NIJDAM J.J., GUO B., FLETCHER D.F. and LANGRISH T.A.G., (2006), “Lagrangian and Eulerian Models for Simulating Turbulent Dispersion and Coalescence of Droplets within a Spray”, *Applied Mathematical Modelling*, **30**(11), 1196-1211.

SUTALO I.D., HARRIS J.A., JORGENSEN F.R.A. and GRAY N.B., (1998a), “Modeling Studies of Fluid Flow Below Flash-Smelting Burners Including Transient Behaviour”, *Metallurgical and Material Transactions B*, **29**(4), 773-784.

SUTALO I.D., JORGENSEN F.R.A. and GRAY, N.B., (1998b), “Experimental and Mathematical Investigation of the Fluid Flow Inside and Below a ¼ Scale Air Model of a Flash Smelting Burner”, *Metallurgical and Materials Transactions B*, **29**(5), 993-1006.

THEMELIS N.J., WU L. and JIAO Q., (1988), “Some Aspects of Mathematical Modeling of Flash Smelting Phenomena”, *Flash Reaction Processes: Center for Pyrometallurgy Conf.*, University of Utah, Salt Lake City, Utah, June 263-285.

VERSTEEG H.K. and MALALASEKERA W., (1995), *An Introduction to Computational Fluid Dynamics: The Finite Volume Method*, Pearson Prentice Hall, Harlow, England.