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# AN ISOTHERMAL MODEL OF AGGLOMERATION IN A FLASH SMELTING REACTION SHAFT

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## ABSTRACT

A steady-state, isothermal model of agglomeration in turbulent, gas-particle flow through a flash smelting reaction shaft is developed. Collisions between pairs of particles are simulated using the turbulent shear kernel of Saffman and Turner (1956). The influence of inlet velocity and turbulence intensity from the burner on collisions and subsequent agglomeration were considered. Increasing the inlet velocity and particle residence time was found to increase agglomeration, while varying the turbulence intensity had only a minimal effect. Examination of the simplifying assumptions is required to improve the comparison of predictions with experimental and other numerical results.

## NOMENCLATURE

$a$ particle agglomeration rate
$c$ particle collision rate
$d$ particle diameter
$D$ diameter dimension
$I$ turbulence intensity
$k$ turbulent kinetic energy
$L$ length dimension
$m_k$ $k$th moment of particle number density
$M$ number of discrete bins/intervals
$n(v)$ particle number density function
$N_i(t)$ particle number density in bin $i$ at time t
$p$ pressure
$s$ discrete domain interval ratio
$S_\phi$ source term of transported variable $\phi$
$t$ time
$\mathbf{u}$ velocity vector with components $(u,v,w)$
$v,x$ particle volume
$v_i$ boundary particle volume between bins $i$ and $i$+1
$v_m$ mean particle volume
$v_s$ scaling particle volume
$x_i$ pivot particle volume for bin $i$

$\delta$ Dirac function
$\varepsilon$ turbulent kinetic energy dissipation rate
$\phi$ general scalar variable
$\mu$ dynamic viscosity
$\rho$ density
$\upsilon$ kinematic viscosity
$\omega$ mass fraction
$\psi$ volume fraction
$\Gamma_\phi$ diffusion coefficient of transported variable $\phi$

## INTRODUCTION

In flash smelting, particles containing metallic sulphides are injected with flux, fuel and oxygen-enriched air through a burner into a reaction shaft where they mix, heat-up, ignite and react. Heat released during exothermic sulphide oxidation reactions causes particles to become molten; these collect at the base of the shaft and are removed once they settle into separate phases. Gaseous products are removed through an offtake shaft. The purpose of the burner is to generate turbulence to mix reactants and improve heat transfer to promote ignition and subsequent reaction. The confined flow of the burner jet results in recirculation of the flow in the shaft. The recirculating flow recycles heat generated in the shaft to heat and ignite the fresh feed. The reaction shaft needs to be long enough to provide sufficient residence time for the particles to be oxidised to the desired extent.

Small particles entrained into the offtake gas stream are defined as dust and are a major operating issue. Dust levels are typically round 5-10w/w% (Davenport, 2001) of the feed stream and this represents a significant loss of product that must be recycled back into the process through the burner, which subsequently decreases throughput. Also, the dust tends to form accretions in and downstream of the offtake shaft, which increases maintenance requirements and downtime.

There are three mechanisms of dust production, denoted here as: (i) mechanical, (ii) chemical, and (iii) physical. Small particles are formed mechanically when larger particles fragment/explode due to the rapid internal build-up of gas from reaction and vapours from evaporation/boiling at the high particle temperatures (eg. Jorgensen, 1985). Small particles are formed by the chemical mechanism when volatile components in the gas phase condense (eg. Jorgensen, 1980). The physical mechanism does not describe the formation of small particles, but instead describes dust production by the entrainment of small particles in the offtake gas that were initially present in the feed.

Work relating to dust in flash smelting has mainly focused on understanding the mechanisms of mechanical (Otero et al., 1991) and chemical (Shook et al., 1995) dust production. The aim of the above mentioned work has been to understand the controlling parameters of the two mechanisms so that operating conditions could be set to minimise dust production by them. However, even if dust production by these two mechanisms were minimised (or even eliminated), the physical mechanism would still remain basically unaffected.

Ojima and co-workers (1986, 1988) investigated reacting particle behaviour using a pilot scale flash smelting furnace operated under industrial conditions. They collected water-quenched particle samples from various locations down the axis of the reaction shaft, and analysed these to determine the extent of reaction and size distribution. Their results indicated the occurrence of agglomeration where the average diameter of the particles increased from about 30 microns in the feed to about 200 microns at the base of the 4m high shaft. They also found that the larger agglomerate particles had reacted to a greater extent. They proposed that larger agglomerate particles had formed from particles that had reacted, heated-up and become molten, and which had then collided and combined with other similarly reacted molten particles. They did not expect un-reacted solid particles to combine upon collision, but rather to bounce off each other instead.

The work of Ojima and co-workers (1986, 1988) seemingly contradicted earlier work by Themelis and Kellogg (1983) who predicted by calculation that particle number densities were too low for collisions (and subsequent agglomeration) to occur in flash smelting.

Themelis et al. (1988) later addressed this contradiction by developing a one-dimensional computer simulation of the flash smelting process that predicted collision and agglomeration of molten particles. Results compared qualitatively well with experimental data and the occurrence of agglomeration of molten particles was clarified. They identified agglomeration as a method of reducing dust production. They also identified the need for further work to establish the behaviour and potential of agglomeration, but there has been no such studies to date.

The aim of this work is to further investigate agglomeration in flash smelting through computer simulation to evaluate its significance in the process.

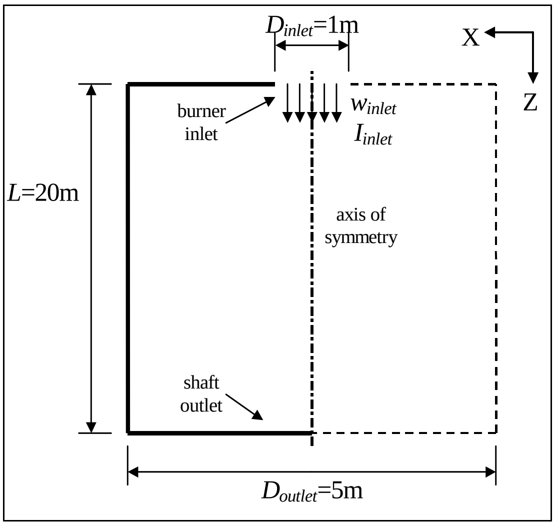


**Figure 1**: Schematic diagram of flash smelting reaction shaft with axi-symmetric mesh geometry.

## THE MODEL

A simplified steady-state model of the flash smelting reaction shaft was developed, featuring two-phase, gas-particle, turbulent flow with agglomeration and mass transfer of the particle phase. The inlet stream of particles was assumed to be molten and mono-dispersed. Reaction and heat transfer were neglected with an isothermal condition of 500K set for the two phases in the inlet stream.

### Phase Transport

The discrete particle phase was assumed to be dilute enough so that its presence did not influence the flow behaviour of the continuous gas phase. Furthermore, the size of the particles was assumed to be small enough so that they followed the gas phase flow behaviour closely, i.e. negligible slip. Based on these assumptions a single flow field was solved for the gas-particle phase mixture.

The mass fraction of the particle phase, $\omega_p$, was solved using the following transport equation;

$$\frac{\partial \rho \omega_p}{\partial t} + \nabla \cdot \left( \rho \mathbf{u} \omega_p \right) = \nabla \cdot \left( \Gamma_{\omega_p} \nabla \left( \omega_p \right) \right) \quad (1)$$

where the diffusion transfer coefficient, $\Gamma_{\omega p}$, was assumed to be dominated by turbulent diffusion with negligible laminar diffusion.

The mass fraction of the gas phase, $\omega_g$, and the phase volume fractions, $\psi_i$, were evaluated as follows;

$$\omega_g = 1 - \omega_p \quad (2)$$

$$\psi_g = \frac{\rho \omega_g}{\rho_g} \quad (3)$$

$$\psi_p = \frac{\rho \omega_p}{\rho_p} \quad (4)$$

The overall density, $\rho$, was evaluated as a phase volume fraction weighted average of phase densities;

$$\rho = \psi_g \rho_g + \psi_p \rho_p \quad (5)$$

The mass flow rate ratio of particles to gas in the feed stream was set to unity.

### Phase Properties

The gas phase was set to have the properties of air, which were evaluated using reference data (Perry and Green, 1997) at the isothermal temperature of 500K to give;

$\rho_g$ = 0.691 kg/m$^3$

$\upsilon_g$ = 3.81$\times$10$^{-5}$ m$^2$/s

The particle phase density was set to be approximately that of a typical sulphide ore as listed in Table 1.

Since the particle phase was assumed to be dilute, the overall kinematic viscosity was assumed to be equal to that of the gas phase, i.e. $\upsilon = \upsilon_g$.

| Particle Phase Parameters | |
|---|---|
| $d$ | 30 microns |
| $\rho_p$ | 5000 kg/m$^3$ |
| $\omega_p$ | 0.5 |
| $\psi_p$ | 1.383×10$^{-4}$ |
| $N_{inlet}(t)$ | 9.78×10$^9$ particles/m$^3$ |
| **DPB Parameters** | |
| $M$ | 5 (bins/intervals) |
| $x_{min}=x_1$ | 1 (scaled using $v_s$) |
| $x_{max}=x_M$ | 16 (scaled using $v_s$) |
| $s$ | 2 |

**Table 1**: Constant parameter values used for each run.

### Turbulent Flow

The continuity and momentum equations were solved for the flow field of the gas-particle phase mixture using the SIMPLEC algorithm for the pressure correction and the boundary log law to evaluate flow near the solid wall boundaries (Versteeg and Malalasekera, 1995).

Turbulence was assumed to be isotropic and was modelled using the two-equation $k$–$\varepsilon$ model of Launder and Spalding (1974) with the turbulent kinematic viscosity was evaluated as follows;

$$\nu_T = 0.09\frac{k^2}{\varepsilon} \qquad (6)$$

Inlet values for $k$ and $\varepsilon$ were evaluated using the following empirical correlations based on the inlet velocity, $w_{inlet}$, and inlet turbulence intensity, $I_{inlet}$, through the burner (Versteeg and Malalasekera, 1995);

$$k_{inlet} = 1.5\left(w_{inlet} I_{inlet}\right)^2 \qquad (7)$$

$$\varepsilon_{inlet} = \frac{0.09^{3/4} k_{inlet}^{3/2}}{0.03 D_{inlet}} \qquad (8)$$

### Agglomeration

Since the particle phase was taken to be dilute, only simultaneous agglomeration between two particles was considered, with simultaneous agglomeration between three or more particles assumed to be negligible.

A population balance equation (PBE) was incorporated into the model to simulate agglomeration. PBE's are used to account for changes in the particle size distribution (PSD) due to discrete events such as agglomeration, and continuous changes such as advection. Ramkrishna (2000) gives the following general form of the PBE where only agglomeration is considered;

$$\frac{\partial n(v,t)}{\partial t} + \nabla\cdot\left(\mathbf{u}n(v,t)\right) - \nabla\cdot\left(\Gamma_{n(v,t)}\nabla\left(n(v,t)\right)\right) = S_{n(v,t)} = S_{n(v,t),b} - S_{n(v,t),d} \qquad (9)$$

where, $n(v,t)$ is the number density function that describes the PSD in terms of the characteristic particle size $v$, which here is set as particle volume.

$S_{n(v,t),b}$ is the agglomeration source/birth term, which accounts for particles of size $v$ forming when two particles of size $v'$ and $v$-$v'$ agglomerate. $S_{n(v,t),d}$ is the agglomeration sink/death term, which accounts for particles of size $v$ disappearing when they agglomerate with another particle of size $v'$ to form a particle of size $v$+$v'$.

Solution methods for PBE's are classified as either (i) continuous (eg. Hamilton et al., 2003), or (ii) discrete (eg. Kumar and Ramkrishna, 1996). Although continuous methods are generally more accurate, they are more complex and more computationally demanding than discrete methods (Hamilton et al., 2003).

The discrete population balance (DPB) fixed-pivot method of Kumar and Ramkrishna (1996) was used to solve the PBE. A discrete method was chosen since the accuracy of a continuous method was considered unnecessary given the other simplifying assumptions already made. Vanni (2000) conducted a review of common discrete methods and found the method of Kumar and Ramkrishna to be simple, robust, generally applicable and computationally efficient.

### Discrete Population Balance

The particle size domain of interest, ($v_{min}$,$v_{max}$), is divided into $M$ number of discrete intervals, denoted as bins. Each bin $i$ spans the domain interval ($v_{i-1}$,$v_i$), which is evaluated as;

$$v_i = s v_{i-1} \qquad (10)$$

with,

$$s = \left(\frac{v_{\max}}{v_{\min}}\right)^{1/M} = \left(\frac{v_M}{v_0}\right)^{1/M} \qquad (11)$$

Each bin $i$ has a fixed-pivot, $x_i$, which is the particle volume assigned to all particles within the bin and is evaluated as;

$$x_i = \frac{2v_i}{1+s} \qquad (12)$$

The particle number density of bin $i$, $N_i(t)$, is assigned to the fixed-pivot volume and is correlated to the overall number density function, $n(v,t)$, as;

$$N_i(t) = \int_{v_{i-1}}^{v_i} n(v,t)\,dv \qquad (13)$$

$$n(v,t) = \sum_{i=1}^{M} N_i(t)\,\delta\left(v - x_i\right) \qquad (14)$$

The set of $N_i(t)$ values combined for each bin $i$ represents a discrete form of the PSD. The DPB simulates changes in the PSD by solving $N_i(t)$ for each bin $i$ using the following transport equation;

$$\frac{\partial N_i(t)}{\partial t} + \nabla\cdot\left(\mathbf{u}N_i(t)\right) - \nabla\cdot\left(\Gamma_{N_i(t)}\nabla\left(N_i(t)\right)\right) = S_{N_i(t)} = S_{N_i(t),b} - S_{N_i(t),d} \qquad (15)$$

The agglomeration source/birth term, $S_{Ni(t),b}$, is given as;

$$S_{N_i(t),b} = \sum_{\substack{j,k \\ x_{i-1}\le x_j + x_k \le x_{i+1}}}^{j\ge k} \left(1 - \tfrac{1}{2}\delta_{j,k}\right)\eta\, a\left(v_j, v_k\right) N_j(t) N_k(t) \qquad (16)$$

with;

$$\delta_{j,k} = \begin{cases} 1 & \text{if } j = k \\ 0 & \text{otherwise} \end{cases} \qquad (17)$$

and,

$$\eta = \begin{cases} \dfrac{x_{i+1} - v}{x_{i+1} - x_i}, & x_i \le v \le x_{i+1} \\[2ex] \dfrac{v - x_{i-1}}{x_i - x_{i-1}}, & x_{i-1} \le v \le x_i \end{cases} \qquad (18)$$

The quantity $\eta$ is an interpolative function that is used to assign new particles that form due to agglomeration to the adjacent fixed-pivot volumes so as to conserve mass and number of particles.

The agglomeration sink/death term, $S_{Ni(t),d}$, is given as;

$$S_{N_i(t),d} = N_i(t)\sum_{k=1}^{M} a\left(v_i, v_k\right) N_k(t) \qquad (19)$$

In the above source terms $a(v,v')$ is the agglomeration rate function which defines the rate of agglomeration of particles of sizes $v$ and $v'$. It is evaluated as the product of the collision rate, $c(v,v')$, and combination efficiency, $e(v,v')$, of particles of sizes $v$ and $v'$.

With the particles being molten, it was assumed that the only requirement of two particles combining is that they collide, and as a result the combination efficiency was set to unity for all colliding pairs of particles, i.e. $e(v,v')$=1.

Turner and Saffman (1956) derived two collision rate expressions due to turbulence, denoted as: (i) turbulent inertia, and (ii) turbulent shearing. Themelis et al. (1988) used the turbulent inertia expression, however, its application is not valid for use here as it was assumed that

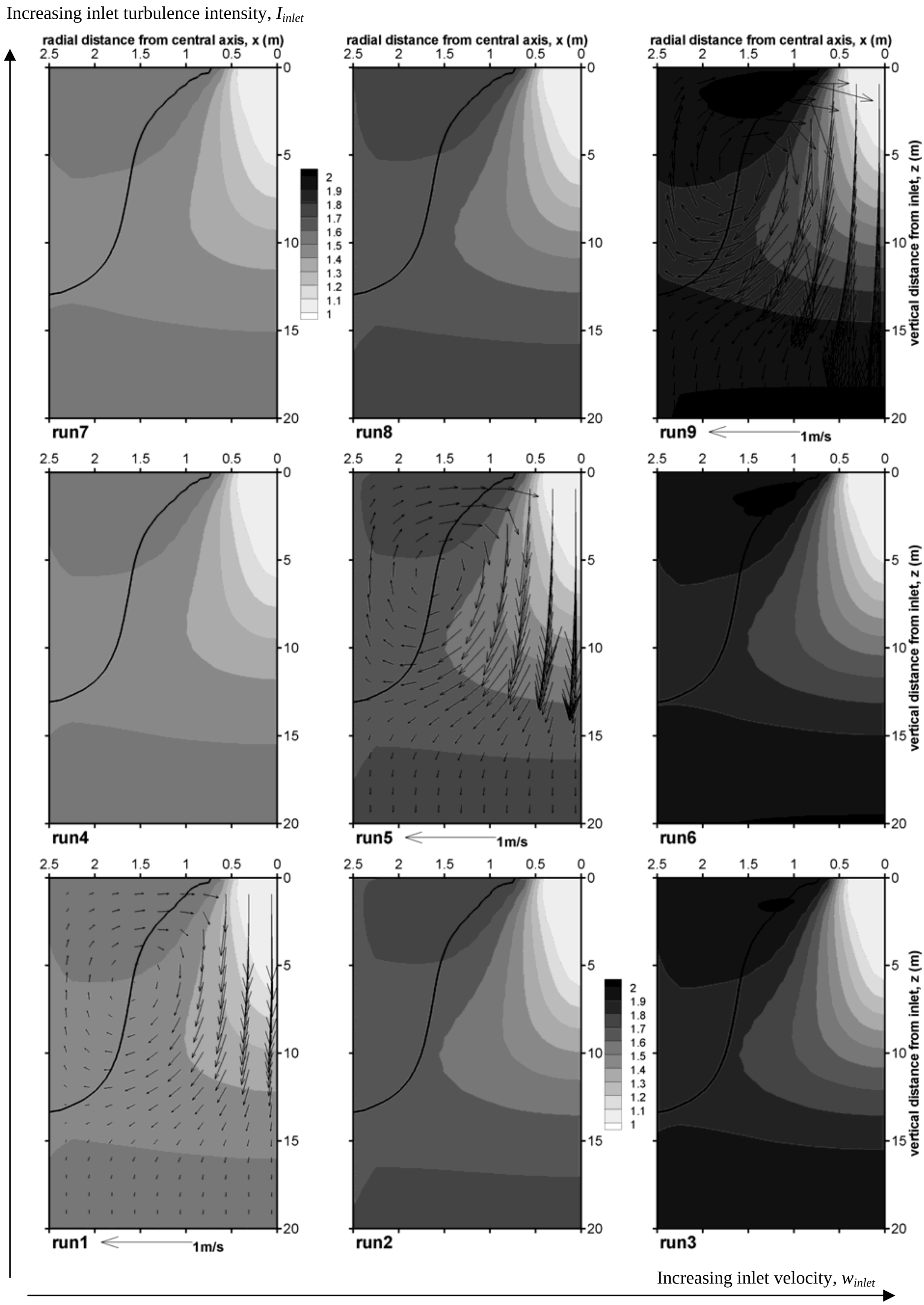


**Figure 2**: Contour plots of mean particle volume throughout reaction shaft for each run listed in Table 2. Vector plots are included to show the flow field for each of the inlet velocities considered. The solid lines included in each plot show the region of zero vertical velocity and are used to indicate the separate recirculation and developing burner jet zones.

the particles have negligible slip. Consequently the turbulent shear expression of Turner and Saffman (1956) was used to evaluate the collision rate, which is given as;

$$c(v_j, v_k) = \sqrt{\frac{8\pi}{15}}\sqrt{\frac{\varepsilon}{\nu}}\left(r_j + r_k\right)^3 \qquad (20)$$

The general moment equation for the *k*-th moment is evaluated as;

$$m_k = \int_0^\infty v^k n(v,t)dv \qquad (21)$$

which can be simplified using equation (14) to give;

$$m_k = \sum_{i=1}^{M} x_i^k N_i(t) \qquad (22)$$

The zero-th, $m_0$, and first, $m_1$, moments evaluate the total number of particles and the total volume of particles, respectively. These were used to evaluate the mean particle volume as follows;

$$v_m = \frac{m_1}{m_0} \qquad (23)$$

## NUMERICAL CONSIDERATIONS

The finite volume method package of PHYSICA was used for the simulations. The Hybrid differencing scheme was employed for advection. Inlet and outlet boundary conditions were set as uniform and constant.

Behaviour was assumed axi-symmetric with a 160 $\times$ 20 mesh constructed for the geometry of dimensions shown in Figure 1. The ratio of outlet diameter to inlet diameter was set to 5:1 and the ratio of shaft length to step height was set to 10:1.

Shaft length was increased until the entire recirculation zone that develops was captured. Mesh element dimensions were set so that the condition of $y^+$<300 was satisfied adjacent to the solid walls. Sensitivity tests with a denser 320 $\times$ 40 mesh show only a typical change in the magnitude of the mean particle volume of about 4%.

The calculation is regarded as having converged to a steady-state solution when the normalised sum of the residuals is less than 0.1% for flow and 0.0001% for DPB.

## RESULTS

Agglomeration in flash smelting was investigated by varying the inlet flow conditions of velocity and turbulence intensity, which independently influenced the level of turbulence and subsequent collision rate (i.e. agglomeration rate) as predicted by equations (7), (8) and (20). Table 1 lists constant parameter values used in each run, while Table 2 lists variable values used for specific runs. The particle number density of the inlet stream, $N_{inlet(t)}$, was evaluated using the inlet mono-dispersed particle diameter and particle volume fraction values. The domain values were scaled/non-dimensionalised with the scaling volume, $v_s$, which was set to the volume of an inlet mono-dispersed particle.

Contour plots of the evolving mean particle volume throughout the reaction shaft for each of the runs in Table 2 are displayed in Figure 2. Vector plots of the flow velocity for each of the inlet velocities is also included to illustrate flow behaviour in relation to particle behaviour.

Recirculation of the flow is clearly observed and is seen to promote agglomeration. This occurs because of increased particle residence time in the recirculation zone. Increasing inlet velocity and inlet turbulence intensity both tend to increase agglomeration but by differing degrees.

| CFD Run | $w_{inlet}$ (m/s) | $I_{inlet}$ | $k_{inlet}$ ($m^2/s^2$) | $\varepsilon_{inlet}$ ($m^2/s^3$) |
|---|---|---|---|---|
| 1 | 5 | 0.05 | $9.38\times10^{-2}$ | $1.57\times10^{-1}$ |
| 2 | 10 | 0.05 | $3.75\times10^{-1}$ | $1.28\times10^{0}$ |
| 3 | 20 | 0.05 | $1.50\times10^{0}$ | $1.01\times10^{1}$ |
| 4 | 5 | 0.10 | $3.75\times10^{-1}$ | $1.28\times10^{0}$ |
| 5 | 10 | 0.10 | $1.50\times10^{0}$ | $1.01\times10^{1}$ |
| 6 | 20 | 0.10 | $6.00\times10^{0}$ | $8.05\times10^{1}$ |
| 7 | 5 | 0.15 | $8.44\times10^{-1}$ | $4.24\times10^{0}$ |
| 8 | 10 | 0.15 | $3.38\times10^{0}$ | $3.40\times10^{1}$ |
| 9 | 20 | 0.15 | $1.35\times10^{1}$ | $2.72\times10^{2}$ |

**Table 2**: Variable values used for specific runs.

## DISCUSSION

The three regions where significant agglomeration is observed in the results shown in Figure 2 are: (i) the shear layers between the inlet and recirculation zones, (ii) the recirculation zone in the top corner of the shaft, and (iii) the outlet at the base of the shaft. The shaft wall region is seen to have negligible affect on agglomeration.

The turbulent shear layers form as the flow profile develops from the uniform inlet flow from the burner. They are responsible for the majority of the agglomeration observed, as indicated by the many narrow contour levels in this region. This finding is in accordance with the collision kernel of Turner and Saffman (1956) used here, where the collision rate is proportional to the turbulence energy dissipation rate, which is highest in the shear layers.

The recirculation zone and the shaft outlet are seen in Figure 2 to be the regions where the particle size peaks. This is a result of particles experiencing a larger residence time in these regions, which gives them more chance to agglomerate.

Increasing the inlet velocity will decrease overall particle residence times in the system, which will tend to decrease overall agglomeration. However, the opposite is observed in Figure 2 with the peak scaled particle sizes increasing from approximately 1.6 to 2.0 (+25%) for an increase in inlet velocity of 5 to 20 m/s (+300%). This indicates that the increased level of turbulence generated by the increased inlet velocity has a more substantial effect on agglomeration than the decreased residence time.

Figure 2 shows that while the inlet velocity has a strong effect on agglomeration, increasing the inlet turbulence intensity only marginally increases agglomeration. This is because the flow and turbulence behaviour within the shaft were found to be relatively insensitive to the inlet turbulence intensities considered.

Under the conditions examined the scaled mean particle volume is seen to reach a maximum of double the inlet mono-dispersed particle volume at the highest inlet velocity of 20 m/s. This is equivalent to approximately a 25% increase in particle diameter.

Comparison of results with that of the experimental work of Ojima and co-workers (1986, 1988) and the numerical results of Themelis et al. (1988) are poor. Reasons for this discrepancy may be a result of some of the simplifying assumptions made here.

The assumption that the particles experience negligible slip is a significant one, which if relaxed would possibly result in less agglomeration in the recirculation zone of entrained particles and more agglomeration down the shaft by falling particles. Inclusion of particle slip would also enable the use of the turbulent inertia collision rate expression as derived by Saffman and Turner (1956), which predicts a higher rate of agglomeration for a similar pair of particles than the turbulent shear expression used here. Themelis et al. (1988) used this collision rate expression, which may in part explain differences in predictions.

The assumption of molten particles at the inlet is not considered too unrealistic as particles are found to heat at high rates of around $10^4$K/s (Jorgensen, 2001), which would mean they became molten soon after entry.

Jorgensen et al. (1992) reviewed various techniques used for collecting particle and gas samples from the flash smelting process. The collection of water-quenched particle samples as used by Ojima and co-workers (1986, 1988) was discussed where it was stated that the technique possibly favoured the collection of larger particles due to the evolution of steam that diverted small particles away. This tends to generate false agglomeration in the results due to the collection of only larger particles, and is proposed as a possible reason in part to explain the differences in the predictions in this work with the experimental results of Ojima and co-workers (1986, 1988).

## CONCLUSION

A simplified, steady-state, isothermal, gas-particle, turbulent flow model with a discrete population model has been developed to investigate agglomeration of molten particles in the reaction shaft of a flash smelter. Significant agglomeration was observed with the majority of it occurring in the shear layers generated by the developing flow from the burner into the reaction shaft. Results showed agglomeration to be promoted by increased inlet velocity and increased particle residence time. Increasing the inlet turbulence intensity had minimal effect on agglomeration. The mean particle volume was found to double under the highest inlet velocity considered. Further work is required to examine the underlying assumptions of the model to improve predictions of agglomeration in comparison with experimental and other numerical results.


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