

# Turbulence Modulation by Mass Exchange in a Model of a Flash Furnace Gas-Particle Jet

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## ABSTRACT

When mass transfer occurs between the particle and gas phases of a turbulent two-phase flow, the net gain or loss to the gas fraction may influence turbulent dispersion. In a flash smelting reaction, there is a net gain of mass to the gas phase which could result in an enhancement of dispersion through the transfer of turbulent kinetic energy from the particles. The importance of the effect is assessed here for flow of a confined gas-particle jet in a geometry which models a laboratory scale, single inlet flash furnace shaft. Flow is assumed to be hot, but isothermal, so that mass transfer can be isolated from complicating effects of heat transfer. Two way coupling models are adapted to include the effect of interphase mass exchange on turbulence. Flow calculations predict that the effect is negligible in this case.

## NOMENCLATURE

$C$	concentration (mass/volume) of $O_2$
$d_p$	particle diameter
$D$	shaft diameter
$D_g$	effective diffusion coefficient of $O_2$
$D_{O_2}$	laminar diffusion coefficient of $O_2$
$D_t$	turbulent diffusion coefficient of $O_2$
$F_p$	instantaneous drag
$J_c$	mass/volume/time of $O_2$ consumed
$J_e$	mass/volume/time of $SO_2$ created
$k$	turbulent kinetic energy of gas
$k_0$	$k$ without particles
$k_m$	mass transfer coefficient (velocity)
$m$	particle/gas mass fraction
$n$	parameter in equations (9) & (10)
$Re_p$	particle Reynolds number
$S_k$	extra dissipation in the $k$ equation

$S_\epsilon$	extra dissipation in the $\epsilon$ equation
$Sc$	Schmidt number
$Sh$	Sherwood number
$t_p$	particle relaxation time
$u$	instantaneous gas velocity
$U$	mean gas phase velocity
$v$	instantaneous particle phase velocity
$V$	mean particle phase velocity
$U_{in}$	inlet gas velocity
$w$	defined by equation (13)
$x$	axial coordinate from the inlet

## Greek symbols

$\beta$	factor in equation (6)
$\epsilon$	turbulence dissipation rate
$\epsilon_0$	$\epsilon$ without particles
$\theta$	particle volume fraction
$\mu$	laminar gas viscosity
$\mu_t$	eddy viscosity of the gas
$\mu_{t0}$	eddy viscosity of gas without particles
$\rho$	density of gas
$\rho_s$	density of solids
$\bar{\rho}_p$	bulk density of particle phase

## 1. INTRODUCTION

In flash smelting, particulate concentrates containing nickel or copper sulphides, flux and fuel are injected with oxygen-enriched air into a reaction shaft located vertically below the inlet. The flow in the reaction shaft forms a confined jet in which the concentrate ignites and sulphur is removed by oxidation. This process is enhanced by recirculation and dispersion of particles which increases particle exposure to oxygen and heat. Thus furnace operation depends significantly on the fluid dynamics of the particle-laden

gas jet.

Gas-phase turbulence can be affected profoundly by the presence of particles (Humphrey, 1990). This has important implications for the dispersion of particles, momentum, heat and gaseous components within the reaction shaft. For particle/gas mass fractions of order unity (volumetric solids fraction  $\sim 10^{-3}$ ), a two-way coupling occurs between the particles and the turbulence. In particular, small particles increase the turbulence dissipation rate due to relative velocity fluctuations between the gas and particles (Hetsroni, 1989; Gore and Crowe, 1989). This results in a lower turbulent diffusivity in the gas. A detailed discussion of particle-turbulence interaction and the modelling of particle-laden flows is given in recent reviews by Crowe (1993), Elghobashi (1994), and Crowe *et al.* (1996).

For a system in which mass transfer occurs between the particle and gas phases (e.g. in chemical reaction or evaporation/condensation), the net gain or loss to the gas fraction can further influence the turbulence. In flash smelting,  $O_2$  is consumed and  $SO_2$  is created with a net gain of mass to the gas phase which may result in an enhancement of turbulence (and hence dispersion) through the transfer of turbulent kinetic energy from the particles. This effect has not been studied within the context of flash smelting, and its importance is not known. In a different context, Mostafa and Mongia (1987) numerically modelled evaporating sprays taking turbulence modulation by interphase mass transfer into account, but they did not quantify the contribution of the effect in their overall prediction.

Hahn and Sohn (1990) and Jorgensen *et al.* (1995) developed comprehensive numerical models of the flash smelting process including chemical reaction kinetics, and heat and mass transfer. Turbulence was represented by the standard two-equation  $k - \epsilon$  model with the gas phase eddy viscosity modified to depend on the particle loading according to an empirical expression proposed Melville and Bray (1979). No account or assessment was taken of turbulence modification by interphase mass transfer.

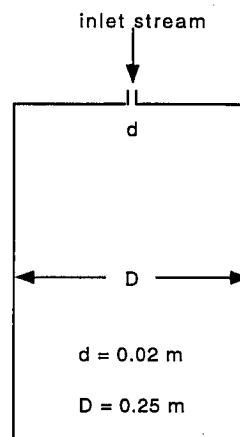


Figure 1: Schematic of the cylindrical flow geometry

An approach to modelling gas-particle turbulent interaction, which is more systematic than that of Melville and Bray (1979), is based on the development of the  $k$  and  $\epsilon$  equations from the instantaneous momentum equations. Two such coupling models are those of Chen and Wood (1985) and Tu and Fletcher (1994). Additional source/sink terms, which derive from the instantaneous drag force, occur in both turbulence equations. Additional terms, which derive from the instantaneous momentum exchange due to interphase mass transfer will also occur in general. Very recently, Davidson (1997) compared numerical flow predictions, without mass transfer, based on the two-way coupling models of Melville and Bray (M & B), Chen and Wood (C & W), and Tu and Fletcher (T & F) for isothermal, non-reacting confined jets.

The aim of the present paper is to adapt the M & B, C & W, and T & F two-way coupling models to include the effect of interphase mass exchange on turbulence, and to use numerical flow predictions to assess the importance of that effect. Flow is assumed to be hot, but isothermal, so that the mass transfer can be considered in isolation from the complicating effects of heat transfer. Confined jet flow in a single inlet cylindrical geometry (similar to the laboratory scale, flash furnace shaft described by Hahn and Sohn, 1990, Table VII) is considered, as shown in Figure 1.

## 2. THE MODEL

A simplified model which incorporates mass transfer due to chemical reaction without an associated treatment of heat transfer assumes:

- (i) uniform gas and particle temperatures
- (ii) instantaneous ignition of particles.

These conditions will be most closely met for small particles and very high gas temperatures. The ignition temperature is about 500 – 800 K. Here we assume a gas temperature of 1500 K, approximately equal to the melting point of concentrate particles (Asaki *et al.*, 1985). In practice this might be achieved by the additional injection of oil particles into the shaft. Nguyen *et al.* (1992) have shown that combustion of the oil rapidly raises the particle temperature to about 1500 K with the temperature rise being much faster for 75  $\mu\text{m}$  particles than for 200  $\mu\text{m}$  particles.

Hahn and Sohn (1990) noted that the variation in particle size within the reaction shaft is uncertain. In their model, they allowed the size to vary with the extent of reaction. In contrast, Jorgensen *et al.* (1995) chose a fixed particle size but varied the density. Here, particle size and density are assumed to be unchanged by processes within the shaft. This allows the convenient use of an Eulerian description of the particle phase.

An Eulerian two-phase model provides a formal structure for averaging procedures required to deal with turbulent interactions. The Reynolds-averaged form of the governing equations of motion, describing the conservation of mass and momentum of each phase is based on that of Adeniji-Fashola and Chen (1990), modified for mass transfer. The volume fraction ( $\theta$ ) of particles is taken to be small and the total gas volume fraction approximated by unity. The pressure gradient is assumed to act only on the gas phase. The mass/volume/time of  $\text{O}_2$  consumed and  $\text{SO}_2$  created are denoted by  $J_c$  and  $J_e$ , respectively.  $\text{O}_2$  leaves the gas phase by reacting with the solid phase which, in turn, releases  $\text{SO}_2$  into the gas phase. Changes to the density of the gas phase resulting from mass exchange are ignored (i.e.  $\rho$  is

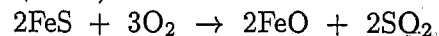
taken as fixed). Details of the corresponding flow equations without mass exchange are given elsewhere (Davidson, 1997). Mass exchange introduces additional source terms  $J_e \mathbf{V} - J_c \mathbf{U}$  and  $J_e - J_c$  in the gas phase momentum and continuity equations, respectively, with identical terms of opposite sign in the particulate phase momentum and continuity equations.

The transport equation for oxygen is

$$\nabla \cdot (\mathbf{U}C) = \nabla \cdot (D_g \nabla C) - J_c \quad (1)$$

where  $C$  denotes the concentration (mass/volume) of  $\text{O}_2$ . The effective diffusion coefficient of  $\text{O}_2$  in the turbulent flow field is given by  $D_g = D_{\text{O}_2} + D_t$ .

For molten concentrate particles, the typical and dominant reaction is (Asaki *et al.*, 1985)



The reaction releases two moles of  $\text{SO}_2$  for every three moles of  $\text{O}_2$  consumed. Since the molecular weights of  $\text{SO}_2$  and  $\text{O}_2$  are 64 and 32, respectively, then

$$J_e = \frac{4}{3} J_c \quad (2)$$

showing that there is a net mass gain to the gas phase. The reaction is controlled by the rate of oxygen diffusion to the particle (Hahn and Sohn, 1990; Jorgensen *et al.*, 1995) whereby

$$J_c = \frac{6k_m \theta C}{d_p} \quad (3)$$

assuming spherical particles. The mass transfer coefficient  $k_m$  is determined from the Ranz and Marshall (1952) empirical correlation for the Sherwood number:

$$Sh = 2 + 0.6Re_p^{1/2} Sc^{1/3} \quad (4)$$

where  $Sh = k_m d_p / D_{\text{O}_2}$ .

### 2.1. Two-way Coupling

The extra dissipation terms appearing in the  $k$  and  $\epsilon$  equations, and denoted here by  $S_k$  and  $S_\epsilon$ , derive from correlations involving fluctuations in the instantaneous drag force

( $F_p$ ) and interphase mass transfer contribution to momentum ( $J_e \mathbf{v} - J_c \mathbf{u}$ ). Kinetic energy is lost from the gas phase because of friction between particles and the gas during turbulent fluctuations. When mass exchange occurs between the phases, gas phase kinetic energy is gained or lost depending on the direction of the mass exchange.

The standard relation for drag exerted by spherical particles on the gas is

$$\mathbf{F}_p = (1 + 0.15 Re_p^{0.687}) \frac{\bar{\rho}_p}{t_p} (\mathbf{v} - \mathbf{u}) \quad (5)$$

where  $t_p = d_p^2 \rho_s / 18\mu$  is the particle relaxation time, and the particle Reynolds number  $Re_p = \rho d_p |\mathbf{v} - \mathbf{u}| / \mu$ .

The term  $S_k$ , for example, becomes

$$S_k = -\frac{\beta}{t_p} \bar{\rho}_p (2k - \overline{u'_i v'_i}) - (2J_c k - J_e \overline{u'_i v'_i}) \quad (6)$$

where  $\beta = 1 + 0.15 \overline{Re}_p^{0.687}$ . In deriving equation (6), a triple correlation has been ignored as well as fluctuations in  $J_c$ ,  $J_e$ , and  $\rho_p$ .

Extending the Chen and Wood (1985) two-way coupling model to include the factor  $\beta$  and the interphase mass transfer effect gives

$$S_k = -2k\beta \frac{\bar{\rho}_p}{t_p} (1 - \exp(-0.5t_p \epsilon / k)) - 2k(J_c - J_e \exp(-0.5t_p \epsilon / k)) \quad (7)$$

$$S_\epsilon = -2\epsilon(\beta \frac{\bar{\rho}_p}{t_p} + J_c) \quad (8)$$

Note that for  $J_c = J_e = 0$  (zero interphase mass transfer), equations (7) and (8) reduce to those published by Chen and Wood (1985).

Similarly extending the corresponding Tu and Fletcher (1994) model of  $S_k$  and  $S_\epsilon$  (again including  $\beta$  and interphase mass transfer) yields

$$S_k = -2k\beta \frac{\bar{\rho}_p}{t_p} (1 - \exp(-0.09 \frac{t_p \epsilon}{m^n k})) - 2k(J_c - J_e \exp(-0.09 \frac{t_p \epsilon}{m^n k})) \quad (9)$$

$$S_\epsilon = -2\epsilon\beta \frac{\bar{\rho}_p}{t_p} (1 - \exp(-0.4 \frac{t_p \epsilon}{m^n k})) - 2\epsilon(J_c - J_e \exp(-0.4 \frac{t_p \epsilon}{m^n k})) \quad (10)$$

where  $n = 0$  for  $m \leq 1$  and  $n = 1$  for  $m > 1$ . Equations (9) and (10) with  $J_c = J_e = 0$  were shown by Tu and Fletcher to give improved predictions for vertical pipe flow with  $m > 1$  where  $m$  was defined as the ratio of the particle to gas mass flow rate. In the present paper  $m$  is defined as  $m = \bar{\rho}_p / \rho$  and equations (9) and (10) are implemented with this definition of  $m$  applied locally.

A two-way coupling model based on Melville and Bray (1979) sets  $S_k = S_\epsilon = 0$  but evaluates the eddy viscosity  $\mu_t$  of the particle-laden gas empirically as a fraction of the eddy viscosity  $\mu_{t0}$  without particles as

$$\mu_t = \frac{\mu_{t0}}{(1 + \bar{\rho}_p / \rho)^{0.5}} \quad (11)$$

when there is no interphase mass transfer. In that case, the Chen and Wood two-way coupling can be reduced to the Melville and Bray equation (11) for very small particles (Davidson, 1997). Underlying this result is the assumption that production and dissipation of turbulent kinetic energy are equal, and the characteristic length scale ( $k^{3/2} / \epsilon$ ) of turbulent eddies is the same with or without particles (Gore and Crowe, 1989). These assumptions can also be applied to derive the following expression, similar to equation (11), for non-zero interphase mass transfer:

$$\frac{\mu}{\mu_{t0}} = \frac{(1 + \bar{\rho}_p / \rho)^{-0.5}}{w + (1 + w^2)^{0.5}} \quad (12)$$

$$w = \frac{(J_c - J_e) k_0}{\rho(1 + \bar{\rho}_p / \rho)^{0.5} \epsilon_0} \quad (13)$$

Note that equation (12) reduces to equation (11) when interphase mass transfer is absent, as required.

Equation (12) shows that for  $J_c < J_e$  (net mass transfer into the gas phase), mass exchange tends to increase the eddy viscosity, and hence turbulent dispersion. This is the circumstance for flash smelting. The converse applies when  $J_c > J_e$ . When  $J_c = J_e$ , no effect due to mass exchange is predicted by equation (12). This occurs because the gas and particle velocities are equal in the limit of very small particles in which case there is no net transfer of kinetic energy due to mass exchange when  $J_c = J_e$ .

The factor  $k_0/\epsilon_0$  in equation (13) is an eddy time scale. For the present case this is estimated approximately as 0.01 seconds based on a fluctuating velocity of  $0.1U_{in}$  and eddy length scale of  $0.1D$ . Using this estimate gives  $w \sim 0.05$  for  $50 \mu\text{m}$  particles and  $w \sim 1$  for  $10 \mu\text{m}$  particles (based on a particle/gas mass fraction  $m = 1$ ,  $\rho_s = 4300 \text{ kg/m}^3$ ,  $\rho = 0.235 \text{ kg/m}^3$  and  $D_{O_2} = 2.3 \times 10^{-4} \text{ m}^2/\text{s}$  at 1500 K). Thus we expect interphase mass transfer to have a negligible effect for  $50 \mu\text{m}$  particles, with the possibility that it may be important for smaller particle sizes in the inlet region where particle concentrations are highest.

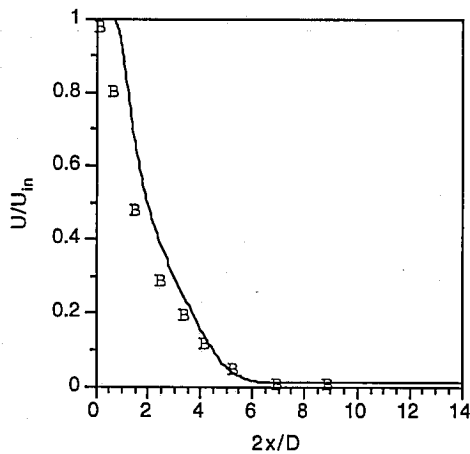


Figure 2: Predicted and experimental centreline axial velocities of single phase gas flow in a 121:1 area expansion. The symbols denote experimental data of Morrison *et al.* (1988).

### 3. NUMERICAL CONSIDERATIONS

A finite volume method is used to solve the discretised flow equations, incorporating the modified  $k$  and  $\epsilon$  equations, on a non-uniform staggered grid. Particle concentrations are small at solid boundaries, so standard log law boundary conditions are applied for the gas phase and free slip is assumed for the particle phase there. At the inlet, the particle velocity is taken to be 0.2 of the gas velocity (20 m/s at 1500 K) with assumed uniform velocity profiles, consistent

with Hahn and Sohn (1990). The inlet turbulence intensity is taken to be 0.04, and the inlet oxygen fraction is taken as 0.2. At the flow exit, axial gradients of variables are taken to be zero.

Hybrid first-order upwind/central differencing is applied in an iteration procedure based on the SIMPLE algorithm (Patankar, 1980). A  $155 \times 47$  numerical grid is used in a flow geometry with a length/diameter ratio of 4.5. Comparison of results with predictions based on skew upwind differencing (Raithby, 1976), which reduces false diffusion, were negligible for selected test cases. The calculation is regarded as having converged to a steady state when the normalised sum of the residuals of each transport equation is less than 0.1 per cent.

## 4. RESULTS AND DISCUSSION

### 4.1. Comparison with Experimental Data

The flow geometry considered (Figure 1) consists of an expansion with an area ratio of 156:1. Flow prediction for such a high aspect ratio is first tested against the single phase (gas only) data of Morrison *et al.* (1988) who measured velocities in an expansion with an area ratio of 121:1. The agreement between predicted and experimental centreline velocities is shown to be very acceptable in Figure 2.

For a gas-particle jet in a sudden expansion, Hardalupan *et al.* (1992) reported velocity measurements for a 25:1 area ratio. The author is not aware of similar data for larger area ratios more representative of that in Figure 1. In Figure 3, predicted centreline gas and particle velocities corresponding to the experiment of Hardalupan *et al.* (1992), for which  $m = 0.14$ , show an adequate agreement with the measured values for each two-way coupling model, with the M & B model giving the best agreement. Similar agreement between the predictions of the two-way coupling models is found for the geometry in Figure 1 when  $m = 0.2$  and  $m = 1$ . However, for  $m = 5$  the corresponding predictions are substantially different with an

apparently anomalous M & B prediction of reverse flow at the outlet. However, the M & B model is only expected to be valid for  $m \leq O(1)$  (Melville and Bray, 1979). Since the T & F two-way coupling model gives improved predictions for  $m > 1$ , at least in the case of upward pipe flow, it will be used hereafter.

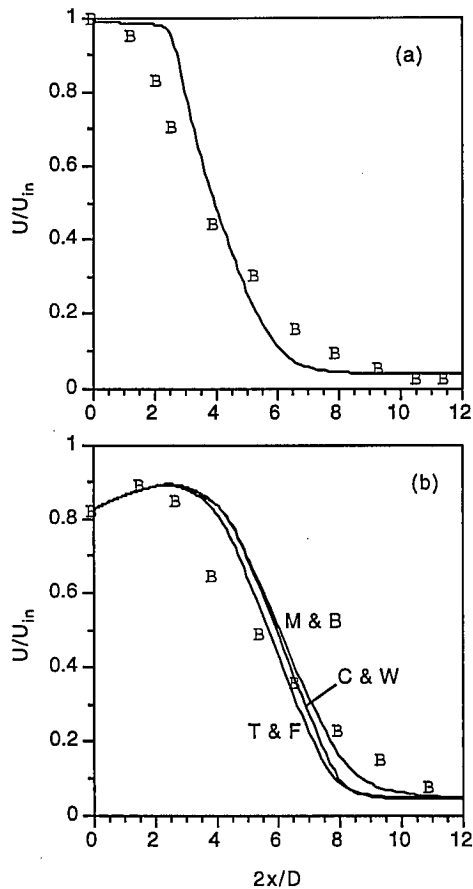


Figure 3: Predicted and experimental centerline axial velocities of (a) single phase gas flow and (b) 40 micron particles in gas-particle flow for a 25:1 area expansion and an inlet mass fraction of 0.14. Predictions are based on the Melville and Bray (M & B), Chen and Wood (C & W), and Tu and Fletcher (T & F) two-way coupling models. The symbols denote experimental data of Hardalupan *et al.* (1992).

#### 4.2. Predictions

The predicted effect on the axial particle velocity with and without mass exchange is shown in Figure 4. Each particle velocity

has the scaled value of 0.2 at the inlet. Velocities predicted when mass exchange is included lie slightly above the corresponding values without mass exchange. (The velocity increase is due to the increased gas volume caused by the reaction). The effect of mass exchange comprises the contribution of the exchange terms in the momentum and continuity equations together with the contribution to particle-turbulence two-way coupling. The combined effect on the velocity is seen to be small for the cases considered (mass fractions 5 and 50, particle diameters 10 and 50  $\mu\text{m}$ ). The predicted velocity difference due to turbulence modulation by mass exchange is even smaller.

The predicted oxygen fraction along the axis (Fig. 5) shows a fall in concentration due to reaction. Note that the immediate drop in the predicted oxygen concentration from its inlet value occurs because ignition of particles is assumed to be instantaneous. The more rapid fall for 10  $\mu\text{m}$  particles occurs because their total surface area is greater than for 50  $\mu\text{m}$  particles at the same mass loading. Recalculating the flow with the mass exchange contribution to turbulence removed yields almost identical results. However, in Section 2 a rough estimate, based on equations (12) and (13) for the eddy viscosity, indicated that the effect may be important for 10  $\mu\text{m}$  particles. The reason for this discrepancy is the rapid drop in the oxygen fraction predicted for this case when the estimate is calculated using inlet parameters.

#### 5. CONCLUSION

Flow of a gas-particle jet in a sudden expansion (156:1) is investigated numerically for a simplified single-entry, cylindrical model of a flash furnace shaft, assuming hot isothermal flow and instantaneous ignition of particles.

The two-way coupling models of Melville and Bray (1979), Chen and Wood (1985), and Tu and Fletcher (1994) are adapted to include the effect of interphase mass exchange on turbulence. In particular, a new modified form of the eddy viscosity of Melville and Bray is presented.

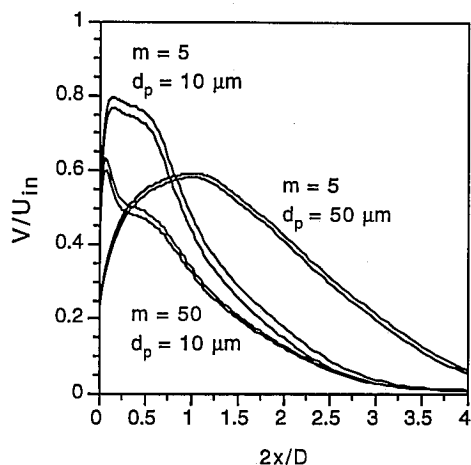


Figure 4: Predicted axial particle velocity, with and without mass exchange, in the flash furnace geometry shown in Figure 1 for two different inlet particle/gas mass fractions and particle diameters. Velocities are scaled by the inlet gas velocity. Calculations are based the Tu and Fletcher (T & F) two-way coupling model.

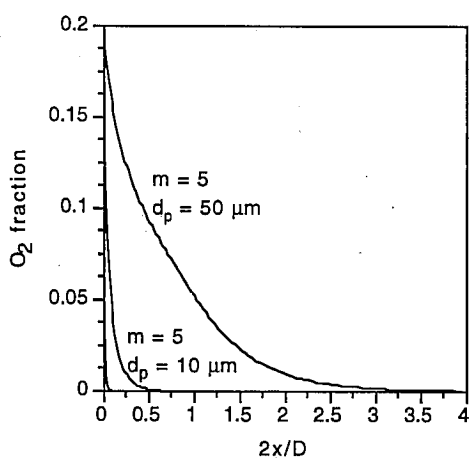


Figure 5: Predicted axial oxygen fraction in the flash furnace geometry shown in Figure 1 for two different inlet particle/gas mass fractions and particle diameters with mass exchange occurring. Calculations are based the Tu and Fletcher (T & F) two-way coupling model.

Flow calculation of the flash furnace jet with reaction (and hence interphase mass exchange) using the modified Tu and Fletcher model predicted that the reaction had little effect on the flow fields for combinations of mass fractions (5 and 50) and particle size (10 and 50  $\mu\text{m}$ ); however, the predicted

oxygen concentration showed a rapid drop downstream consistent with expected results following particle ignition. The interphase mass exchange contribution to turbulence was shown to have no noticeable effect on the predicted oxygen concentration on the axis in this case. This contradicts the conclusion derived from an estimate of the modified Melville and Bray eddy viscosity; however, that estimate was based on the inlet value of the oxygen concentration rather than a downstream value which is much lower.

Despite the conclusion that interphase mass exchange has almost no effect on the flow field and oxygen concentration in the present idealised flash furnace shaft model, it may yet prove to be important in other applications involving mass transfer in gas-particle flows if the mass exchange rates are large enough. Provided the exchange rates in such applications can be expressed in terms of local flow variables, the modified two-way coupling models can be applied to incorporate the mass exchange effect.

## 6. ACKNOWLEDGMENT

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