TOWARDS SONIC INJECTION IN PEIRCE-SMITH CONVERTERS: A COMPUTATIONAL
FLUID DYNAMICS (CFD) MODELLING STUDY

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ABSTRACT

This research work forms part of an assessment to complement the feasibility of implementing
high pressure sonic injection into relatively small (2.25 m I.D by 3.66 m I.L) Peirce-Smith converters
(PSC) used at Lonmin Plc. Work has been carried out to characterize the fluid dynamics of three-phase
(air, matte and slag) fluid flow in these converters using Computational Fluid Dynamics (CFD) simulations.
The investigation has been done to study the flow pattern of the three phase system at high air pressure
injection achieving sonic velocity at the tuyere exit into the converter. The 2-D and 3-D simulations of
the three phase system were carried out using the volume of fluid (VOF) and realizable $k-\varepsilon$ turbulence
models to account for the multiphase and turbulence nature of the flow, respectively. These models were
implemented using the commercial CFD numerical code FLUENT. A detailed study of the flow pattern
has been presented in the form of contour plots and the results obtained are useful for understanding plume
extension and velocity distribution, shear wall stress distribution, and phase distribution characteristics in
the system. The results provide a basis for further development of sonic injection technology into
relatively small industrial Peirce-Smith converters with the ultimate objective of achieving lower energy
consumption, improved process efficiency and increased throughput of the converting process.
INTRODUCTION

Peirce-Smith converters (PSC) have been used in copper (Cu) and nickel (Ni) making smelters for more than a century for the purpose of removing iron (Fe) and sulphur (S) chemically associated with copper-nickel mattes through exothermic oxidation reactions. This process is commonly referred to as conversion. In principle, conversion is a submerged injection process, where typically air (or oxygen enriched air), at subsonic velocity (typically < 150 m/s), is laterally blown into liquid matte (Cu-Ni-Fe-S system). Oxygen preferentially reacts with Fe and S to produce iron oxide (FeO), which is slagged off, and sulphur dioxide (SO₂), which reports to the process off gas.

Despite a long standing period of operational existence, the mode and principle of operation has remained unchanged. The major change that has come to the design is the inception of different versions of the typical PSC, notably the Hoboken-type converter, which is fitted with a siphon that allows process gas to be collected without atmospheric dilution (Bustos, Cardoen and Janssens, 1995). As fairly expressed by Hoechele and Brimacombe (1979) at the time they were studying alternative injection mechanism for submerged injection processes, the unaltered principle of operation is more of a “consequence of history and conservatism than technological limitations.”

In recent years, small versions of typical copper-nickel PSC have been used in Platinum Group Metals (PGMs) smelters for the same purpose of removing Fe and S chemically associated with Cu-Ni mattes rich in PGMs. Lunnin Plc is one such smelter operating with PSC of approximately one third the working volume of a typical copper-nickel PSC. Based on subsonic flow conditions currently employed in these PSC operations, common and deleterious problems have been experienced, namely tuyere blockage requiring continuous punching operation, high refractory wear in the tuyere region leading to converter campaign life averaging 30 days after reline, and substantial splattering and splashing causing operational downtime with intermittent off-stack periods for cleaning the converter mouth and aisle. In addition, oxygen efficiency as low as 65% has been observed, which is attributed to the punching operation as a result of substantial amounts of air losses due to leakages.

The conversion process occurs at high temperature (> 1,100 °C) in a steel shell and refractory lined vessel which preclude visual observation and experimentation. To understand key process aspects, and hence prospects of re-engineering, physical and numerical modelling techniques have been developed and conducted. Physical models with different types of fluids simulating matte (some simulating slag) in PSC were developed to study the gas behaviour in the tuyere proximity, splashing occurrences, mixing, phase distribution and mass transfer phenomena (Hoechele and Brimacombe, 1979; Richards, Legeard, Bustos, Brimacombe and Jorgensen, 1986; Chibwe, Akdogan and Eksteen, 2011; Chibwe, Akdogan, Aldrich and Eric, 2011; Chibwe, Akdogan, Aldrich and Taskinen, 2011).

In a study to investigate splashing in PSC, Richards et al. (1986) concluded that development and intensification of slopping resulting from the manifestation of a unimodal wave was the main cause of splashing. Quantitative analysis given in their water model based study showed that gas–liquid coupling increases with tuyere submergence, hence the reduction in splashing. For the small working volume PSC used in the PGMs industry, tuyere submergence is low (~ 405 mm) relative to the one achievable in Cu-Ni PSC (Brimacombe, Meredith and Lee, 1984). In this regard, any possible injection consideration in the small PSC should take this limitation into account.

PSC campaign life is dependent on the integrity and state of the refractory in the converter. Due to subsonic flow conditions, the refractory in the tuyere line has commonly been observed to deteriorate much faster than the rest of the converter. Some research on the mechanism of refractory wear has been carried out and published (Goni, Barbes, Bazan, Brandleze, Parra and Gonzalez, 2006; Gonzales, Calle and Drew, 2007). Three mechanisms of refractory wear have been identified, namely chemical corrosion, thermal spalling, and mechanical wear (Gonzalez et al., 2007). Based on a Nodal Wear Model (NWM), which is a thermo-chemical based numerical model, Goni et al. (2006) quantitatively evaluated at 35% to 65% the ratio of refractory wear in a PSC due to chemical and thermo-mechanical processes. The thermo-
mechanical form of refractory erosion is due to a combination of gas dynamics in the proximity of the tuyere nozzle, where high temperature gradients exist, and the punching operation, which generates mechanical shock. In the last three decades, efforts have been directed to non-adapted under-expanded (choked) flow injection into PSC, which achieves jetting conditions at the tuyere exit. In this operation, the tuyere exit velocity of the injected gas into the bath is sonic and the gas exits as highly unstable bubbles with a high degree of fragmentation, breaking up into small bubbles and therefore increasing the air–liquid interfacial area, which potentially increases the oxygen utilization.

Supersonic and sonic flow operations were first conceived in the steel making industry for the purposes of steel refining. In 1979, Hoefele and Brimacombe carried out the first experimental studies on the possibility of sonic injection into PSC using air–water, air–zinc chloride (ZnCl2), and air–mercury (Hg) systems coupled with plant trials. Pressure measurements in both laboratory and plant showed that only the air–mercury system had the same bubble frequency of 10 to 12 Hz in the laboratory and the plant, indicating the importance of the gas–liquid density ratio on the dynamics of submerged injection processes. Improved penetration of gas into liquid was observed at sonic conditions.

Subsequent plant trials with straight bore tuyeres designed for sonic flow were conducted at the Asarco Tacoma smelter in the USA (Brimacombe et al., 1984), the Toyo smelter in Japan (Kimura, Tsuyuguchi, Ojima, Mori and Ishii, 1986), the Noranda Howe smelter and the Inco Copper Cliff smelter in Canada (Bustos, Brimacombe, Richards, Valded and Pelletier, 1987). These trials utilized between 1 and 4 sonic tuyeres in simultaneous operation with conventional tuyeres and analyzed different sonic injection operation aspects. Major conclusions in these trials were that the horizontal penetration force is lower relative to the buoyancy force exerted by the bath, the stability of the tuyere pipe accretions formed depends on the stage of the converting cycle, and punchless operation is possible at higher injection pressure. In 1987, Bustos et al. gave a qualitative evaluation of refractory wear in the proximity of the tuyeres.

Based on the understanding of accretion formation and stability, coupled with the process benefits of sonic injection operation, the Air Liquide Shrouded Injetor (ALSI) technology was developed (Bustos et al., 1995). With ALSI technology, air oxygen enrichment between 30% and 40% has been achieved without detrimental refractory erosion. ALSI technology was commercial implemented at the Falconbridge (now Xstrata Nickel) smelter in Canada (Bustos, Kapusta, Macnamara and Coffin, 1999) in a nickel PSC, and at the Thai Copper Smelter in Thailand (Pagador, Wachgama, Khuankala and Kapusta, 2009) in a Hoboken-type copper PSC. Detailed design and operation of ALSI is given by Bustos and Kapusta (2000).

Despite the success recorded during sonic injection trials on PSC using single pipe sonic tuyeres, there is no commercial implementation of such operation to date. Loumin Plc envisages implementing such technology on a commercial scale. Prior to implementation, key process aspects need to be evaluated amongst them, slopping, splashing and mixing characteristics, refractory integrity and possible extend of air penetration into the bath in these relatively small converters with shallow tuyere submergence. A realistic representation of such a system needs to be developed in order to have conclusive interpretations. As shown in 1979 by Hoefele and Brimacombe, the air–water system does not give a realistic representation of the high temperature air–liquid system and a rigorous system development satisfying the geometry and dynamic similarity is needed.

Computational Fluid Dynamics (CFD) analysis offers an attractive alternative and has been used successfully in many industrial analysis simulations (Hani, Hui, Kan, You, Pak and Song, 2001; Cervantes-Clemente, Real-Ramirez, Palomar-Pardave, Hoyos-Reyes, Gutierrez-Villegas and Gonzalez-Trejo, 2009; Alam, Naser and Brooks, 2010). The major advantages of CFD application are its cost-effectiveness due to reduced experimental costs as well as its ability to run simulations under controlled conditions. Against such background, in this work, we characterized the fluid dynamics of the three-phase (air, matte and slag) flow in the PSC used at Loumin Plc using CFD simulations. These simulations gave both qualitative and quantitative analysis of flow characteristics in the converter. The investigation was
done to study the flow pattern of the three phase system at higher air pressure injection achieving sonic velocity at the tuyere exit into the converter. The 2-D and 3-D simulations of the three phase system were carried out using the volume of fluid (VOF) and realizable $k-\varepsilon$ turbulence models to account for the multiphase and turbulence nature of the flow, respectively. These models were implemented using the commercial CFD numerical code FLUENT.

**NUMERICAL SIMULATION OF AIR INJECTION**

In this work, 2-D and 3-D simulations were carried out based on a slice model of a Lonmin Plc PSC. Due to mesh densities involved in these simulations, simulation of the entire converter was not feasible. Table 1 gives the dimensions of the actual converter and slice model.

<table>
<thead>
<tr>
<th>Table 1 – Lonmin converter and slice model dimensions</th>
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<tbody>
<tr>
<td><strong>Dimensions</strong></td>
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<tr>
<td>Diameter inside refractory (mm)</td>
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<tr>
<td>Length inside refractory (mm)</td>
</tr>
<tr>
<td>Tuyere inner diameter (mm)</td>
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<tr>
<td>Number of tuyeres</td>
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<tr>
<td>Average tuyere spacing (mm)</td>
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</table>

**Numerical Simulation and Model Description**

The computational domain was discretized into small control surfaces and volumes (for 2-D and 3-D) for calculations. Very fine meshes are necessary to capture accurately the flow pattern. In this work, a multi-size variable mesh was used. Fine mesh elements were employed in the matte–slag domain with the free air region having elements approximately 2.5 times larger. Modelling was done on an Intel® Core™ i7 CPU with a 3.46 GHz processor and 8.0 GB of installed Random Access Memory (RAM). The commercial CFD code ANSYS FLUENT, version 14.0, was used for the calculations on a High Power Computing (HPC) cluster with an installed capacity of eight 2.83 GHz processors per node with 16 GB of RAM.

Based on estimates of matte additions and the transient nature of converting cycles, four stages in the converting cycle period were calculated, with matte and slag heights estimated as given in Table 2.

<table>
<thead>
<tr>
<th>Table 2 – Matte/slag levels estimated distribution</th>
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<tbody>
<tr>
<td><strong>Stage in Cycle</strong></td>
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<td></td>
</tr>
<tr>
<td>Beginning of blow (BTB)</td>
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<tr>
<td>End of first blow (EFB)</td>
</tr>
<tr>
<td>Midway of a typical blow (MTB)</td>
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<tr>
<td>Cu-Ni blow</td>
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</tbody>
</table>

In this paper, simulations conducted at midway of a typical blow (MTB) conditions will be presented as this period accounts for more than 85% of the converting cycle time. The initialized solution revealing the fluid density distribution (air, slag and matte) in the computational domain is shown on Figure 1.
Air flow conditions at the tuyere exit into the bath were calculated based on compressible flow theory. Using the equation used by Suni, Kishimoto, Kikuchi, and Igarashi (2006), the Mach number, \( M \), at the tuyere exit into the bath was calculated using Equation 1.

\[
M = \sqrt{\frac{2}{\gamma-1} \left( \frac{P_a}{P} \right)^{\frac{\gamma+1}{2}} - 1}
\]

In this equation, \( \gamma \left( = \frac{C_p}{C_v} \right) \) is the ratio of specific heat capacities, \( P_a \) (Pa) is the tuyere back pressure, and \( P \) (Pa) is the pressure at the tuyere exit into the bath. In the present study, sonic flow at the tuyere exit with \( M = 1 \) was obtained under the pressure conditions evaluated.

To reduce the computational time during the simulations, the flow in the sonic tuyere was not included but simulated separately, and the flow conditions at the tuyere exit were taken as the inlet boundary condition of the computational domain. This value was calculated using the isentropic flow theory. Only two simulations were conducted with 300 mm tuyere pipe coupled to the converter to see the development of air flow into the converter. A segregated solver with an implicit approach was used to calculate the pressure, velocity, turbulence and density through solving the unsteady and compressible flow conservation governing equations, namely continuity, momentum and energy.

Figure 1 – Computational domain (a) 2-D and (b) 3-D as exported and initialized in FLUENT

**Governing Equations**

The general equations for conservation of mass (continuity), momentum and energy are given by Equations 2, 3 and 4 respectively.

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{v}) = S_{\rho}
\]

\[
\frac{\partial (\rho \vec{v})}{\partial t} + \nabla \cdot (\rho \vec{v} \vec{v}) = \nabla P + \nabla \cdot (\tau) + \rho g + \vec{F}
\]
\[
\frac{\partial}{\partial t}(\rho E) + \nabla \cdot (\bar{v}(\rho E + P)) = \nabla \cdot \left( k_{\text{eff}} \nabla T - \sum_{j} h_j \bar{J}_j + \underbrace{\tau_{\text{eff}} : \bar{v}}_{\text{viscous dissipation}} \right) + S_E
\]

In these equations, \( \rho \) (kg/m\(^3\)) is the density, \( \nabla \) is the partial derivative in all directions with respect to the coordinate system used, \( \bar{v} \) (m/s) is the velocity magnitude, \( S_m \) is the mass added to the continuous phase from the dispersed phase, \( P \) (Pa) is the static pressure, \( \tau \) is the stress tensor, \( \rho g \) is the gravitational body force, \( \vec{F} \) is the external body forces, and \( k_{\text{eff}} \) (W/Km\(^1\)) is the effective thermal conductivity which is the sum of the thermal conductivity and the turbulent thermal conductivity, defined according to the turbulence model being used, and \( \tau_{\text{eff}} \) (Pa) is the effective stress tensor. The first three terms on the right-hand side of Equation 4 represent the energy transfer due to conduction, species diffusion, and viscous dissipation, respectively. \( S_E \) is the energy source term, which includes the heat of chemical reaction and any other volumetric source terms defined in the model and \( E \) (J) is the total energy as described in Equation 5, where \( h \) (J) is the sensible enthalpy.

\[ E = h + \frac{\rho + \bar{v}^2}{2} \]

Models

The Volume of Fluid (VOF) Model

In order to account for the multiphase nature of the flow, the VOF model was used. The interfacial behaviour of air, matte and slag was captured by this model using a compressive discretization scheme. This is accomplished by surface tracking of the phase interfaces in the system through solution of the VOF continuity equation given in Equation 6.

\[ \frac{\partial}{\partial t} (\alpha, \rho) + \nabla \cdot (\alpha, \rho \bar{v}) = S_m \]

In the model, the different phases are treated numerically as interpenetrating continua thus inevitably introducing the concept of phasic volume fraction where the volume fractions in each computational cell sums to unity. In other words, if the \( i \)th fluid volume fraction in the cell is denoted by \( \alpha_i \), then it follows that:

\[ \alpha_i = 0: \quad \text{The computational cell does not contain the } \alpha_i \text{ fluid} \]
\[ \alpha_i = 1: \quad \text{The computational cell is full and contains only the } \alpha_i \text{ fluid} \]
\[ 0 < \alpha_i < 1: \quad \text{The computational cell contains at least a fraction of } \alpha_i \text{ fluid} \]

Based on this formulation, the primary phase volume fraction will be calculated against the constraint given in Equation 7.

\[ \sum_{\alpha} \alpha = 1 \]

The Turbulent Model

Incorporation of the effects of turbulence on the flow field inside the model was accomplished by using the realizable \( k - \varepsilon \) model. This is a two-equation model based on transport equations for the
turbulence kinetic energy, \( k \), and its rate of dissipation, \( \varepsilon \). It is a relatively recent development by Shih, Liou, Shabbir, Yang and Zhu (1995), which offers improvements in the overall energy transfer. Both transport equations for \( k \) and \( \varepsilon \) were derived from exact equations. The turbulence variables \( k \) and \( \varepsilon \) are obtained from the transport Equations (8) and (9), respectively.

\[
\frac{\partial}{\partial t}(\rho k) + \frac{\partial}{\partial x_i}(\rho ku_i) = \frac{\partial}{\partial x_i}\left[ \left( \mu + \frac{\mu_t}{\sigma_k} \right) \frac{\partial k}{\partial x_i} \right] + G_k + G_s - \rho \varepsilon - Y_k + S_k \tag{8}
\]

\[
\frac{\partial}{\partial t}(\rho \varepsilon) + \frac{\partial}{\partial x_i}(\rho \varepsilon u_i) = \frac{\partial}{\partial x_i}\left[ \left( \mu + \frac{\mu_t}{\sigma_\varepsilon} \right) \frac{\partial \varepsilon}{\partial x_i} \right] + \rho C_{\varepsilon} S_{\varepsilon} - \rho \varepsilon \frac{C_{\varepsilon}}{k + \sqrt{\nu \varepsilon}} + C_{\varepsilon} \frac{\varepsilon}{k} C_{\varepsilon} G_k + S_{\varepsilon} \tag{9}
\]

In these equations, \( G_k \) is the generation of turbulence kinetic energy due to the mean velocity gradients, \( G_s \) is the generation of turbulence kinetic energy due to buoyancy, \( Y_k \) is the contribution of the fluctuating dilatation in compressible turbulence to the overall dissipation rate, \( C_{\varepsilon} \), \( C_{\varepsilon x} \), \( C_{\varepsilon y} \) and \( C_{\varepsilon z} \) are constants, and \( \sigma_k \) and \( \sigma_\varepsilon \) are the turbulent Prandtl numbers for \( k \) and \( \varepsilon \), respectively (ANSYS, 2011).

Solution Method

The flow conservation governing equations, the VOF model equations and \( k-\varepsilon \) turbulence model equations (Equations 2 to 9) were solved with FLUENT version 14.0. This package is a finite volume solver using body-fitted computational grids. A coupled algorithm was used for pressure-velocity coupling. A Compressive Interface Capturing Scheme for Arbitrary Meshes (CICSAM) discretization was used to obtain face fluxes, when the computational cell is near the interface using piecewise-linear approach. This scheme was necessary due to the high viscosity ratios involved in this flow problem (ANSYS, 2011). A time step of 0.0001 second was used and found to be sufficient for maintenance of numerical convergence at every time step and stability. Convergence of the numerical solution was determined based on surface monitoring of integrated quantities of bulk flow velocity and turbulence, and scaled residuals of continuity, x-, y-, z-velocities, \( k \) and \( \varepsilon \). The residuals of all quantities were set to \( 10^{-4} \) and the solution was considered converged when all the residuals were less than or equal to the set value.

RESULTS AND DISCUSSION

Plume Extension and Velocity Distribution

In the numerical simulations conducted in this work, the computed plume extensions for current (subsonic) and envisaged (sonic) operation are plotted in Figure 2.

A dimensionless parameter, \( \frac{x}{d_e} \), where \( x \) (mm) is the exit jet distance and \( d_e \) (mm) is the exit tuyere diameter was used to visualize the extend of the plume extension into the converter. The plume extension into the bath for subsonic and sonic conditions is given by \( P_{\text{on}} \) and \( P_{\text{on}} \), respectively. According to our simulation results, \( \frac{P_{\text{on}}}{P_{\text{on}}} \approx 4 \). Extension of the active region into the converter away from the tuyere exit area is essential as it provides an enlarged area for the chemical reactions to take place. In their mass transfer studies in the Peirce-Smith converter, Adjei and Richards (1991) concluded that a substantial part of the chemical reactions in the converter likely occurs in the tuyere region. Vaanm, Pitkälä, Ahokainen and Jokilaakso (1998) also concluded that the most intense conditions for oxidation reactions exist during bubble formation and fragmentation near the tuyere.
Figure 2 – The axial velocity distribution on the tuyere centre axis for subsonic and sonic flow conditions.

Figure 3 – Velocity vector distribution around the tuyere exit at (a) subsonic and (b) sonic flow conditions.

Note: The color scale is different for the two figures: the green color corresponds to about 60 m/s for subsonic while it corresponds to about 180 m/s for sonic.
The simulations also revealed that the bath circulatory velocity outside the plume region is approximately 0.27 m/s for both flow conditions. These results are in agreement with the assumption made by Bustos, Brimacombe and Richards (1988) in their development of a mathematical model for Peirce-Smith converter accretions growth for subsonic and sonic operations. The velocity vector distribution around the tuyere exit for both flow conditions is shown in Figure 3. It can be observed that the sonic injection plume extends further into the bath with a higher velocity (about 180 to 200 m/s) relative to the subsonic operation (maximum of 100 to 120 m/s). Lower velocity regions can easily be seen further away from the plume. Based on these results, it can be concluded that the process efficiency differences observed in lower pressure and higher pressure injection is largely dependent on the oxidation activity around the plume and tuyere exit into the converter as the bulk of the converter behaves in a similar manner in terms of velocity, turbulence and mass transfer as presented by Adjei and Richards (1991).

**Shear Wall Stress Distribution**

The effects of the bath circulation motion and bath density on the walls of the converter were evaluated by calculating the wall shear stress along the converter wall boundaries. According to ANSYS (2011), the wall shear stress (Pa) is defined as:

\[ \tau_w = \rho u_r^2 \]  \hspace{1cm} (10)

In this equation, \( u_r \) (m/s) is the wall friction velocity. Figure 4 shows the wall shear stress distribution for subsonic and sonic flow conditions. Near the tuyeres, for subsonic flow conditions, a maximum wall shear stress of 200 Pa was obtained compared to 125 Pa for sonic flow. This partially suggests a possible mitigation of refractory wear with sonic injection by a lowering of the mechanically induced erosion around the tuyere region.

![Wall shear stress distribution](image)

**Figure 4** – Wall shear stress distribution for subsonic and sonic flow conditions

At the wall in the opposite side of the tuyere line, the stress is slightly higher for sonic injection, possibly due to the propagation of a standing wave at a distance further away from the tuyeres and carrying energy to the opposite side walls relative to the subsonic conditions where energy is instantly dissipated just above the tuyeres as presented in Figure 4.
Figure 5 – Phase distribution density contours (a) at subsonic flow and (b) at sonic flow conditions.
Figure 5 shows the phase density distribution for subsonic and sonic flow conditions. High air volume region in front of the tuyeres can be seen for sonic relative to subsonic flow conditions. This is consistent with the results shown in Figures 2 and 3. Due to the agitation in the regions in front of the tuyeres, a strong emulsification exists creating high reaction rates in the zone. This is in agreement with the observations by Rosales, Fuentes, Ruz and Godoy (1999) in their study of fluid dynamics in a Teniente converter.

CONCLUSIONS

In the present study, we have numerically investigated the behaviour of plume dispersion, velocity distribution, and phase distribution in a relatively small PSC. On the basis of the results and discussions, the main conclusions of this work are the following:

- The injection plume extends into the bath approximately 4 times deeper at sonic flow conditions relative to subsonic flow conditions.
- Under subsonic flow conditions, the injected gas ascends near the converter wall above the tuyeres for a significant period of time, and therefore, a high refractory wear in the tuyere region is expected relative to sonic injection in which the injected gas penetrates further into the bath.
- Wall shear stress values of 200 Pa relative to 125 Pa for subsonic and sonic flow conditions, respectively, suggest a possible prolonged refractory campaign life with sonic injection.
- Higher pressure injection results in high air volume regions in front of the tuyeres relative to low pressure injection operation.
- Process efficiency differences observed in lower pressure and higher pressure injection is largely dependent on the oxidation activity around the plume and tuyere exit into the converter as the bulk of the converter behaves in a similar manner in terms of velocity, turbulence and mass transfer.
- High pressure injection into relatively small PSC is feasible and is likely to increase production and process efficiency.

ACKNOWLEDGEMENTS

The authors wish to acknowledge Lonmin Plc for the financing of this work.

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