A Volume of Fluid (VOF) Method for the Simulation of Metallurgical Flows

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A finite difference numerical method, based on the VOF approach for tracking interface distortions, is presented. It is capable of accurately simulating the fluid flow of multiple immiscible fluids for metallurgical applications. This volume tracking method is based on piecewise linear reconstructions of interfaces, density distributions based on a shifted grid approach, and a fully kernel-based CSF method for surface force modelling. Second order temporal and spatial accuracy are achieved using improved Euler time-stepping enhancement of a two-step projection algorithm, supported by a multigrid-preconditioned GMRES solver that enabled large density ratios (1 : 30 000) between the fluids and fine scale flow phenomena to be resolved. The code was used to simulate the rise of an air bubble in water and in liquid pig iron and was able to capture the time dependent oscillation of the bubble. The bubble velocity varied with the instantaneous shape of the bubble. The averaged terminal velocity of the gas bubble in water was in good agreement with published experimental data. Splash formation from a top submerged gas injection lance was simulated to illustrate the capability of the code in resolving the break up and fragmentation of liquid drops for possible use in the study of bath smelting processes.

KEY WORDS: VOF; bath smelting; numerical modelling; bubble rise; gas injection; splash.

1. Introduction and Previous Work

Incompressible free surface and interfacial fluid flows are an integral part of most natural and industrial processes. In particular, most processes in the metallurgical industry have multiple fluid phases and a free surface present. There is an increasing need to be able to control these complex metallurgical processes and hence, an improved capability to numerically simulate and study these processes. Areas where complex free surface flows present interesting and challenging applications in the metallurgical industry include gas injection, entrainment of mattes and metals in slags, tapping, slopping, skimming of slags, pouring from vessels and ladles,¹⁾ electromagnetic containment,^{2,3)} and plasma spraying.

The finite element approach has been used to model free surface flows in commercial packages, but suffers from the heavy computational load required for remeshing of the moving interfaces. To overcome this problem, Nakayama and Shibata⁴⁾ used a finite element scheme with a density discontinuity to model the free surface that was advected using an upwind scheme. However, the diffusion of the interfaces in their numerical scheme were still quite severe even for simple test cases. Recently, the level set approach of Sussman *et al.*^{5,6)} has been applied for free surface flows. The level set method does not conserve volume and its applicability to complex problems has not been documented.

The use of boundary integral methods gives high resolution of the boundary profile but an arbitrary decision must be made when fluid interfaces break up or coalesce. It is not suitable for cases where extensive fluid fragmentation and coalescence occur. The volume of fluid (VOF) method of Hirt and Nichols⁷⁾ and its extensions^{8–10)} were found to be the most suitable for the development of a generic numerical code to model free surface flows for multi-fluid processing in metallurgical operations.

The VOF method is an Eulerian method that uses a volume fraction indicator to determine the location of the interfaces of different phases in all cells of a computational domain. Although the reconstructed surfaces do not necessarily coincide with the true interface, developments in advection schemes in the last decade have greatly improved the surface resolution. This has enabled the VOF method to model the complex problem of splash generation from impinging drops¹¹⁾ and provide physical insights into parameters that cannot be easily measured experimentally. For the impinging drop, the VOF method combined with surface force modelling based on the Continuum Force approach was able to capture the surface tension effects down to the sub-millimetre level where highly accurate experimental results were available for comparison.¹²⁾ A limitation of VOF-based finite difference algorithms is that for problems involving high density differences, it has traditionally been difficult to perform high fidelity and high resolution simula-

tions as it requires a robust and efficient Poisson equation solver. This has resulted in simulations with the VOF method being limited to small density ratios, normally less than 100. In this paper, we describe a generalised VOF method for multiple fluid flows in metallurgical operations that overcomes this limitation, and have named the code MFVOF (multi-fluid VOF).

2. Governing Equations

The partial differential equations governing the laminar and isothermal flow of incompressible Newtonian fluids are:

- Continuity equation

$$\nabla \cdot \mathbf{U} = 0, \quad \dots\dots\dots(1)$$

- Momentum equation

$$\frac{\partial}{\partial t} \rho \mathbf{U} = -[\nabla \cdot \rho \mathbf{U} \mathbf{U}] - \nabla p + [\nabla \cdot \boldsymbol{\tau}] + \mathbf{F}_b + \mathbf{F}_s, \quad \dots\dots(2)$$

where ρ is fluid density, p is scalar pressure, $\boldsymbol{\tau}$ is the viscous stress tensor, $\mathbf{F}_b$ is a body force, and $\mathbf{F}_s$ is a surface force. In this VOF implementation, the body force was $\rho \mathbf{g}$, the acceleration due to gravity, and the surface force was the surface tension force.

The volume of any fluid species in a mesh cell is described by a fractional volume C whose conservation is given by

$$\frac{\partial C}{\partial t} + \nabla \cdot (\mathbf{U}C) = 0. \quad \dots\dots\dots(3)$$

3. Computational Method

The governing equations were discretised using an Eulerian uniform staggered Marker and Cell (MAC) mesh.¹³⁾ The scalar variables, such as pressure and colour function, are located at the mesh centres, and the vectorial variables, such as velocities, are located at the cell edges. MFVOF was designed to handle 2-D and axisymmetric coordinates. The equations were solved with a second-order improved Euler time-stepping scheme which involved repetition of the two-step algorithm by Chorin¹⁴⁾ at a half time-step and a full time-step. This is similar to a midpoint method and offers second order accuracy. This two-step projection method proceeds as follows:

1. Determine the distribution of the fluid throughout the flow domain at the time step $n + 1/2$

$$C^{n+1/2} = C^n - \frac{\delta t}{2} \nabla \cdot (\mathbf{U}^n C^n). \quad \dots\dots\dots(4)$$

2. Evaluate the density and viscosity distributions based on the new C values. For two fluids this gives

$$\rho^{n+1/2} = \rho_1 C^{n+1/2} + \rho_2 (1 - C^{n+1/2}), \quad \dots\dots\dots(5)$$

$$\mu^{n+1/2} = \mu_1 C^{n+1/2} + \mu_2 (1 - C^{n+1/2}). \quad \dots\dots\dots(6)$$

3. Evaluate the surface tension force $\mathbf{F}_s^{n+1/2}$ using surface curvature estimates based on the C distribution.
4. Find an intermediate velocity field $\mathbf{U}^*$ using the pressure field at time n and half time step $\delta t/2$.

$$\mathbf{U}^* = \mathbf{U}^n + \frac{\delta t}{2} \left[-\nabla \cdot (\mathbf{U} \mathbf{U})^n - \frac{\nabla P^n}{\rho^n} + \mathbf{g} + \frac{\mathbf{F}_s^n}{\rho^n} + \frac{\nabla \cdot \boldsymbol{\tau}^n}{\rho^n} \right]. \quad \dots\dots\dots(7)$$

5. Calculate the pressure correction δP , from the discrete form of the following equation, for time n to $n + 1/2$

$$\nabla \cdot \left(\frac{1}{\rho^n} \nabla \delta P \right) = \frac{2}{\delta t} \nabla \cdot \mathbf{U}^*. \quad \dots\dots\dots(8)$$

6. Update the velocity field and pressure distribution to time $n + 1/2$

$$\begin{aligned} \mathbf{U}^{n+1/2} &= \mathbf{U}^* - \frac{\delta t}{2} \frac{1}{\rho^n} \nabla \delta P, \\ P^{n+1/2} &= P^n + \delta P. \end{aligned} \quad \dots\dots\dots(9)$$

7. Determine the distribution of the fluid throughout the flow domain at the time step $n + 1$

$$C^{n+1} = C^n - \delta t \nabla \cdot (\mathbf{U}^{n+1/2} C^n). \quad \dots\dots\dots(10)$$

8. Evaluate the density and viscosity distributions based on the new C values. For two fluids this gives

$$\rho^{n+1} = \rho_1 C^{n+1} + \rho_2 (1 - C^{n+1}), \quad \dots\dots\dots(11)$$

$$\mu^{n+1} = \mu_1 C^{n+1} + \mu_2 (1 - C^{n+1}). \quad \dots\dots\dots(12)$$

9. Evaluate the surface tension force $\mathbf{F}_s^{n+1}$ using surface curvature estimates based on the C distribution.
10. Find an initial estimate of the velocity field $\mathbf{U}^*$ using the solutions at time $n + 1/2$ and full time step δt .

$$\begin{aligned} \mathbf{U}^* &= \mathbf{U}^n + \delta t \left[-\nabla \cdot (\mathbf{U} \mathbf{U})^{n+1/2} - \frac{\nabla P^{n+1/2}}{\rho^{n+1/2}} + \mathbf{g} + \frac{\mathbf{F}_s^{n+1/2}}{\rho^{n+1/2}} \right. \\ &\quad \left. + \frac{\nabla \cdot \boldsymbol{\tau}^{n+1/2}}{\rho^{n+1/2}} \right]. \end{aligned} \quad \dots\dots\dots(13)$$

11. Calculate the pressure correction δP , from the discrete form of the following equation, for time $n + 1/2$ to $n + 1$

$$\nabla \cdot \left(\frac{1}{\rho^{n+1/2}} \nabla \delta P \right) = \frac{1}{\delta t} \nabla \cdot \mathbf{U}^*. \quad \dots\dots\dots(14)$$

12. Update velocity and pressure fields to time $n + 1$

$$\begin{aligned} \mathbf{U}^{n+1} &= \mathbf{U}^* - \delta t \frac{1}{\rho^{n+1/2}} \nabla \delta P, \\ P^{n+1} &= P^{n+1/2} + \delta P. \end{aligned} \quad \dots\dots\dots(15)$$

It is not possible to use $C^{n+1/2}$ in the source term on the right-hand side of the C advection Eq. (10) because of the geometric nature of the flux calculation. However, because the Youngs' fluxes are estimates of the average values of the fractional volume fluxed over the edge of a cell during time dt , they may be considered time-centred. Thus, the use of C^n in the source terms in Eq. (10) in the second step does not reduce the order of the time integration.

3.1. Advection of the Colour Function C

The piecewise linear interface calculation (PLIC) approach of Youngs¹⁵⁾ was used to update C to follow deformations of fluid bodies as a result of the bulk flow of the fluids. It has been shown by Rudman⁸⁾ to maintain sharp interfaces between fluid bodies and to be superior to the original VOF method of Hirt and Nichols.⁷⁾ Fluxes of individual fluid species across the cell edges are based on approximate reconstructions of the interfaces in each mesh cell.

For a two fluid system, a line segment interface divides an interface cell into two polygonal regions, one fluid i occupying C^i fraction of the cell and the other fluid occupying $1 - C^i$ fraction of the cell. These line segments are oriented to approximate the interface location within the mesh cell such that they are tangential to the outward normal vector $\mathbf{n}$

$$\mathbf{n} = n^r \hat{\mathbf{j}} + n^z \hat{\mathbf{k}} \quad (16)$$

where n^r and n^z are the radial and axial components of the normal vector. The outward normal vector $\mathbf{n}$ is computed from the C distribution using

$$\mathbf{n} = -\nabla C \quad (17)$$

The computation of n^r and n^z for the cell (j, k) is carried out with a finite difference stencil used in the RIPPLE code.¹⁶⁾

$$n_{j,k}^r = \frac{c_{j+1,k+1} + 2c_{j+1,k} + c_{j+1,k-1} - c_{j-1,k+1} - 2c_{j-1,k} - c_{j-1,k-1}}{\delta r} \quad (18)$$

$$n_{j,k}^z = \frac{c_{j+1,k+1} + 2c_{j,k+1} + c_{j-1,k+1} - c_{j+1,k-1} - 2c_{j,k-1} - c_{j-1,k-1}}{\delta z} \quad (19)$$

The angle the outward normal vector makes with the positive r axis, β , is computed from the relative magnitudes of the normal vector components

$$\beta = \tan^{-1} \left(\frac{n^z}{n^r} \right) \quad (20)$$

Fluid i in cell (j, k) occupies a volume (modulo 2π in cylindrical coordinates and $r_j = 1$ for 2D Cartesian coordinates)

$$V_{\text{actual},j,k}^i = C_{j,k}^i r_j \delta r \delta z \quad (21)$$

The exact position of the line segment in the cell is determined by shifting the line segment in a direction parallel to the outward normal vector to create a polygon that encloses the volume $V_{\text{actual},j,k}^i$. The volume of the polygon in cylindrical coordinates (modulo 2π) is

$$V_{pj,k}^i = \frac{1}{6} \sum_{s=1}^t (r_s r_{s+1}) (r_s z_{s+1} + r_{s+1} z_s), \quad (22)$$

and in 2-D Cartesian coordinates is

$$V_{pj,k}^i = \frac{1}{2} \sum_{s=1}^t (r_s z_{s+1} - r_{s+1} z_s), \quad (23)$$

Fig. 1. The fluid interface within an interface cell (i, j) is calculated by a Newton-Raphson iterative method. The interface is moved parallel to the normal and the volume of the fluid is calculated at each estimate. The Newton-Raphson method is second order and normally converges within 2-3 iterations.

Fig. 2. Calculation of the fluid species to the right of the flux line to be fluxed out through the right cell wall using Youngs method. The amount of species i that is fluxed is obtained after the interface is reconstructed geometrically.

where (r_s, z_s) , $s = 1, \dots, t$ are the vertices of the polygon. A Newton-Raphson iterative process, with an under-relaxation factor of 0.5 and a tolerance of 10^{-6} to 10^{-8} of V_{actual} , is used to converge to V_{actual} . Figure 1 shows how the iteration process works.

After the line segment interface reconstructions have been completed for all cells, the fluxes of fluid i are calculated. Only the outward fluxes are computed, while the inward fluxes are obtained from the interface reconstructions in adjacent cells (for which fluxes are outward).

Figure 2 shows an example of fluid fluxed outwards across the right cell-edge in timestep δt for cell (j, k) with velocities (u, w) in the (r, z) directions respectively. The total volume of material fluxed out across this cell-edge is

$2\pi\delta z r_{j+1/2} u_{j+1/2,k} \delta t$. A ‘flux line’ of distance d from the right cell-edge can be drawn to delineate fluid fluxed across the right edge in δt from fluid which remains in the cell. The total volume of material fluxed out across the right cell-edge is $\pi\delta t(r_{j+1/2}^2 - (r_{j+1/2} - d)^2)$. The distance from the flux line to the edge across which fluid is fluxed outward, d , is computed by combining the two alternative volume expressions. For fluxes across each wall of a mesh cell, the distance d is computed as

$$\text{left edge} \quad d = -r_{j-1/2} \left(1 - \sqrt{\frac{1 - 2u_{j-1/2,k} \delta t}{r_{j-1/2}}} \right), \dots (24)$$

$$\text{right edge} \quad d = r_{j+1/2} \left(1 - \sqrt{\frac{1 - 2u_{j+1/2,k} \delta t}{r_{j+1/2}}} \right), \dots (25)$$

$$\text{bottom edge} \quad d = -w_{j,k-1/2} \delta t, \dots (26)$$

$$\text{top edge} \quad d = w_{j,k+1/2} \delta t, \dots (27)$$

The flux of fluid i outward across an edge during δt , F^i , is the volume (on the edge-side of the flux line) bordered by the flux line, the line-segment interface reconstruction, and the edges of the mesh cell. For two dimensional flow problems, the scheme requires fluxing out of the horizontal and vertical cell-edges simultaneously. Direction splitting is used to extend the single dimension approach described above. The radial fluxes are computed first, giving an intermediate volume of fluid i in cell (j, k) after the radial sweep as

$$V_{j,k}^{i*} = (r_j \delta r \delta z) C_{j,k}^i - (F_{j+1/2,k}^i - F_{j-1/2,k}^i), \dots (28)$$

The total fluxes across the right and left walls are different. The apparent total volume of the mesh cell after the radial sweep is

$$V_{j,k}^* = (r_j \delta r \delta z) - r_j \delta z (u_{j+1/2,k} - u_{j-1/2,k}), \dots (29)$$

An intermediate colour function C^{i*} is given by

$$C_{j,k}^{i*} = \frac{V_{j,k}^{i*}}{V_{j,k}^*}, \dots (30)$$

which never exceeds unity. A second axial sweep is then conducted, using the intermediate colour function values, to complete the colour function update from time n to $n+1$.

$$C_{j,k}^{i,n+1} = C_{j,k}^{i*} + \frac{F_{j,k-1/2}^i - F_{j,k+1/2}^i}{r_j \delta r \delta z}, \dots (31)$$

On completion of the update from time n to $n+1$, the volumetric distortion of cell (j, k) predicted by the apparent total volume is corrected. The sweeping is alternated to avoid systematic error build-up.

3.2. Updating the Physical Properties

Volume-weighted averaging calculation of the properties uses the colour function distribution that is located at mesh cell centres. However, accurate estimates of the physical property values at cell-edges are required for computation. This is important for the density because poor cell-edge density estimates result in poor approximations of the continuity of momentum across the interface, for which large

density ratios can lead to instability. A ‘shifted-grid’ approach is used to obtain the values of the density at cell-edges in preference to the averaging of cell-centred density values.

The shifted-grid approach involves computing densities at cell-edge locations based on the volume-average formula used in Eqs. (4) and (5), but using values of C computed at cell edges ($C_{j+1/2,k}$ and $C_{j,k+1/2}$). These cell-edge distributions of C are determined from the cell-centre values by advecting the C distribution defined at cell centres with a uniform velocity field and an (artificial) time-step of Courant number 0.5. As an example, advection of the cell-centre C distribution with the velocity field

$$\tilde{\mathbf{U}} = 0.5 \frac{\delta r}{\delta t} \hat{\mathbf{j}} + 0 \hat{\mathbf{k}} \dots (32)$$

is used to calculate the uniform advection of C half a mesh cell right using the same Youngs-VOF scheme as used in the numerical method for normal C advection. The result is $\tilde{C}$, computed as

$$\tilde{C} = C - \delta t \nabla \cdot (\tilde{\mathbf{U}} C), \dots (33)$$

which is the colour function distribution defined at control volumes centered at $(j+1/2, k)$. The cell-edge estimate of C is extracted from $\tilde{C}$ as

$$C_{j+1/2,k} = \tilde{C}_{j+1,k}, \dots (34)$$

Density estimates at $(j+1/2, k)$ are subsequently computed as done with Eqs. (4) and (5). The shifted-grid approach with Youngs'-VOF results in more accurate approximations of cell-edge densities than the use of arithmetic or harmonic averaging of cell-centre values. This increased accuracy requires the volume-tracking algorithm to execute an additional four times per timestep. Cell vertex viscosities are computed using the harmonic mean averaging of cell-centred viscosity values, which avoids excessive accelerations in less dense, less viscous fluid regions near interfaces.

3.3. Linear Solver

To solve the linear algebra system generated by the Poisson equation, a number of algebra solvers were tested.¹⁷⁾ They include the multigrid (MG), conjugate gradient (CG) and generalised minimum residual (GMRES) methods. A new linear solver, MGGMRES (multigrid generalised minimum residual) was developed, that uses a multigrid method for preconditioning the linear algebra system before solving with the GMRES algorithm.¹⁷⁾ The multigrid preconditioner is based on the defect-correction Galerkin multigrid solver developed by Rudman⁸⁾ and adapted from Wesseling.¹⁸⁾ The multigrid solver is fast but not necessarily robust. Using the multigrid method as a preconditioner in a right preconditioned GMRES method¹⁹⁾ resulted in scalability and low iteration counts. The details of the new solver has been given by Liovic *et al.*¹⁷⁾

3.3. Other Issues

The non-linear momentum advection term in the momentum update (steps 4 and 10 of the solution algorithm) are discretised using the van Leer scheme.²⁰⁾ Second order centred differencing is used to discretise the conservative

form of the viscous stress term ($\nabla \cdot \tau$). The surface tension is modelled using the continuum surface force (CSF) model of Brackbill *et al.*²¹⁾ but the finite difference approximations are replaced by fully kernel based approximations as detailed by Rudman,⁸⁾ which have been shown to reduce the effects of grid-based noise on modelling accuracy.

Lances, weirs and non-standard shapes found in metallurgical vessels are modelled through the use of obstacles. A staircase approach is used to model flow obstacles within the computational flow domain. Entire mesh cells are flagged to lie either within the fluid or within the obstacle. For non-rectangular objects, this approach approximates the object with increasing accuracy as the number of mesh cells is increased.

The flow domain, for problems of interest, is bounded by three types of boundaries: inflow, outflow and solid wall boundaries. Solid wall boundary conditions are applied to obstacle walls. The inflow boundary condition is set by specifying an inlet velocity. For the outflow boundary conditions, the approach of Sani and Gresho²²⁾ is used to ensure a well-posed open boundary condition. At the solid walls at the edge of the flow domain or at the obstacle, the boundary condition can be free-slip or no-slip. At no-slip walls, the normal and tangential components of the velocity are set to zero

$$\mathbf{U} \cdot \hat{\mathbf{n}} = \mathbf{U} \cdot \hat{\mathbf{t}} = 0. \quad (35)$$

where $\hat{\mathbf{n}}$ and $\hat{\mathbf{t}}$ are the unit normal and tangent vectors. Zero normal velocities are set at the wall cells, and zero tangential velocities are enforced using linear interpolation. For free-slip walls, the normal velocity and the tangential stress are set to zero

$$\mathbf{U} \cdot \hat{\mathbf{n}} = (\nabla \mathbf{U}) \cdot \hat{\mathbf{t}} = 0. \quad (36)$$

Zero normal velocities are enforced as for no-slip walls while the zero tangential stress reduces to a homogeneous Neumann boundary condition on the tangential velocity. For velocity components on the walls of cells at the corners of obstacles, the boundary condition on the normal velocity takes precedence over any on the tangential velocity.

Turbulence is not explicitly modelled in MFVOF at present. Turbulence models suitable for VOF calculations of multiphase flows are currently being developed. However, for the cases presented here, the bubble rise occurs in a laminar flow and the start-up of top submerged gas injection begins with a quiescent bath. Nevertheless simulation of gas injection and multi-fluid flow over long time intervals will require turbulence to be incorporated as it develops in the flow. Boris²³⁾ has argued that the monotonic, flux-limited advection scheme can play the role of an implicit sub-grid scale turbulence model in the context of Large Eddy Simulation. In limiting fluxes so that no new minima or maxima are introduced, monotonic flux limiting is designed to destroy the build-up of energy in the smallest re-

solved scales in a physically meaningful way. This limiting flux manifests itself in the resolved-scale flow through an increase in the effective viscosity, and represents the dissipation of resolved-scale kinetic energy. The dissipation of energy from the resolved-scale eddies to the subgrid-scales eddies is therefore modelled in an empirical way. In reality there is also a transfer of energy from the sub-grid scale to the resolved scale, but this cannot be modelled by such a simple framework.

4. Simulation of Bubble Rise

Extensive validation and verification tests of the MFVOF code have been performed on a wide range of standard test problems. Physical problems used to validate the code include the formation of waves, bubbles and splash, top submerged gas injection, bubble rise, and entrainment from multiple liquid layers overflowing a weir. Details of these tests can be found in Liovic's PhD thesis.²⁴⁾ Examples of MFVOF's ability to deal with large density differences are given here for an air bubble rising in water, an air bubble rising in pig iron and splash formation by a top submerged lance.

4.1. Air Bubbles in Water

The MFVOF code was used to simulate the rise of single axisymmetric air bubbles in water as experimental data on the various bubble sizes and shapes have been published.²⁵⁻²⁷⁾ The density ratio of air to water is 1:997. The shapes of the air bubbles are characterised by the Eötvös number, Eo , the Morton number M , and the bubble Reynolds number, Re , defined as

$$Eo = g(\rho_l - \rho_g)d_c^2/\sigma \quad (37)$$

$$M = g\mu^4(\rho_l - \rho_g)/(\rho_l^2\sigma^3) \quad (38)$$

$$Re = d_c u_T \rho_l / \mu \quad (39)$$

where d_c is the equivalent bubble diameter, σ is the surface tension, μ is the liquid viscosity, and u_T is the terminal velocity. Clift *et al.*²⁶⁾ provides a graphical correlation of the dimensionless numbers with the bubble shape. The bubble sizes simulated are shown in Table 1.

The terminal velocities for the Reynolds number were based on the correlation given in Clift *et al.*²⁶⁾ for the air-water system at 20°C,

$$u_T = \sqrt{2.14 \frac{\sigma}{\rho_l d_c} + 0.505 g d_c} \quad (40)$$

All three cases are classified by Clift *et al.*²⁶⁾ to be in the wobbling regime. However, for $Re < 1000$, the onset of oscillations is delayed, while the largest bubble is close to the spherical cap regime. A mesh of 96 horizontal cells and

Table 1. Conditions and results for the simulation of air bubbles rising in water.

Equivalent bubble diameter (mm)	Eo	M	Re	Regime Clift <i>et al.</i> ²⁵⁾	u_T (m/s)	$u_{num.}$ (m/s)
3	1.2	$10^{-10.6}$	773	wobbling	0.260	0.267
6	4.8	$10^{-10.6}$	1409	wobbling	0.237	0.233
12	19.1	$10^{-10.6}$	3208	wobbling	0.269	unstable

Fig. 3. Shape of air bubbles in water starting from rest for different equivalent bubble diameters. The final resulting shape or instability is independent of whether the bubble starts from a spherical or elliptical shape. The 12 mm case is scaled at half the size of the 3 and 6 mm cases. The time intervals are 0.01 s for the 3 and 6 mm cases, and 0.02 s for the 12 mm case.

960 vertical cells was used to represent an equivalent container of 4 by 40 bubble diameters respectively. Numerical tests showed that at 4 bubble diameters, the container wall had little effect on the bubble rise velocity. Grid independence was obtained with a grid of 64 by 640 mesh cells but the 96 by 960 mesh cells grid was used to provide better resolution of the bubble contours. The boundary conditions at the container wall were set as free slip. **Figures 3 and 4** show the bubble shapes and rise velocities respectively.

The 3 mm bubble shows very small shape oscillations that are seen in the small velocity variations at steady state. However, the velocity variations are small and the averaged terminal velocity reached within 0.1 s is in good agreement with the prediction of Eq. (40). The aspect ratio varied from 0.35 to 0.37 due to small variation in the shape and compares well with the value of 0.36 measured in the experimental study of Aybers and Tapucu.²⁷⁾

For the 6 mm bubble, the shape begins oscillating soon after the bubble begins rising, resulting in a periodic behaviour. The simulation shows a small bubble pinching off at the very early stages of bubble rise but the extreme oscillations damp out after the first oscillation and settles down to a periodic behaviour as shown by the velocity profile. In the periodic behaviour regime, the averaged velocity agrees well with the prediction of Eq. (40). Nevertheless, an axisymmetric simulation may not provide a good representation of the bubble behaviour as an experimental study by

Fig. 4. Velocity of air bubbles in water starting from rest for different equivalent bubble diameters. The 12 mm case shows that the bubble decelerates as it spirals outwards during breakup.

Morton and Liow²⁸⁾ showed that air bubbles of this size and larger exhibit 3-D oscillations and are rarely axisymmetric in shape.

For the 12 mm bubble, the shape oscillations are strong enough that the bubble breaks up within one oscillation period. In contrast, Clift *et al.*²⁶⁾ predicts a wobbling bubble close to the spherical cap regime. At the high *Eo* number above 20, Han and Tryggvason²⁹⁾ have shown that liquid drops break up as the drop viscosity and surface tension decreases and the stability is dependent on the Eötvös number. Our VOF simulations agree with the numerical work of Han and Tryggvason in predicting the drop is unstable in the axisymmetric configuration. Experimentally, air bubbles of this size are three dimensional in nature and their interface can be stabilised by small amounts of surface molecules. Such surface molecules act to increase the surface tension of the gas-liquid interface. Hence for higher surface tension values, it can be expected that the gas bubble will be stable in the axisymmetric configuration to larger diameters as is the case for the air-pig iron case discussed next.

4.2. Air Bubble in Pig Iron

In this series of simulations, the air is taken to be in thermal equilibrium with the pig iron at 1 200°C. The air density used is 0.232 kg/m³ and pig iron density is 7 000 kg/m³, giving a density ratio of air to pig iron of 1:30 000. Pig iron viscosity is taken as 0.007 kg/(m·s), and surface tension as 1.265 N/m. Equation (40) was used to estimate the terminal velocity although it is not known how suitable the equation is for liquids other than water. Nevertheless, the estimates obtained were in good agreement with the fluid-independent regime map in Clift *et al.*²⁶⁾ The bubble sizes simulated are shown in **Table 2**.

The bubble shapes and velocities are given in **Figs. 5 and 6** respectively. The numerical simulations are stable at this high density ratio and predict that the bubbles do not break up during rise. The bubbles are more rounded than the air-water case for an equivalent bubble diameter the equivalent Eötvös number is lower since the higher surface tension stabilises the bubble interface. For the 3 mm bubble, the as-

Table 2. Conditions and results for the simulation of air bubbles rising in pig iron.

Equivalent bubble diameter (mm)	Eo	M	Re	Regime Clift <i>et al.</i> ²⁵⁾	u_T (m/s)	$u_{num.}$ (m/s)
3	0.5	$10^{-11.8}$	1137	wobbling	0.379	0.381
6	2.0	$10^{-11.8}$	1842	wobbling	0.307	0.313
12	7.8	$10^{-11.8}$	3636	wobbling	0.303	0.298

Fig. 5. Shape of air bubbles in pig iron starting from rest for different equivalent bubble diameters. The 12 mm case is scaled at half the size of the 3 and 6 mm cases. The time intervals are 0.01 s for the 3 and 6 mm cases, and 0.02 s for the 12 mm case.

Fig. 6. Velocity of air bubbles in pig iron starting from rest for different equivalent bubble diameters.

pect ratio varies between 0.53 to 0.54 compared to 0.36 for the air–water case. The 6 mm bubble does not oscillate as much as for the similar air–water case. For the 12 mm bub-

Fig. 7. Schematic of the dimensions for the simulation of top submerged air injection into water.

ble, the oscillations are quite large but the bubble remains intact. Grid noise is more noticeable with the higher surface tension but does not destabilise the calculation. The estimated terminal velocity is comparable to the calculated average terminal velocity. The velocity profiles show much more variation than for the air–water case. The oscillations damp out for the 3 mm case, are larger and periodic for the 6 mm case but non-periodic for the 12 mm case.

5. Splash Formation by a Top Submerged Lance in an Axisymmetric Vessel

Figure 7 shows the physical dimensions of the top-submerged gas injection process that was simulated with a 128×384 mesh, the mesh cells having a vertical/horizontal aspect ratio of 1.4 : 1. The use of a lance to vessel diameter ratio of 1 : 8 in a circular bath scales geometrically with the lance to vessel diameter ratio in the Ausmelt furnace.³⁰⁾ Air was injected downward through the lance at a constant flow rate of 0.7 l/s, corresponding to a mean gas inlet velocity of 1.0 m/s. The lance was submerged 100 mm into the water. The time step in the simulation was restricted using a Courant number of 0.25, and instantaneous flow fields were captured from the simulation at a rate of 100 per second. The simulated interfacial profile throughout the computational flow domain was extracted from the colour function distribution by the contour $C=0.5$.

Figure 8 shows the instantaneous interfacial profiles generated by the simulation from startup to 1.24 s into the simulation. As these are axisymmetric simulations, the profiles in Fig. 8 were generated by mirroring the results at the

Fig. 8. Time sequence of the fluid flow for the simulation of top submerged air injection into water. Water and air are coloured black and white respectively.

centerline to give a complete cross-sectional view. The inertia of the gas results in the initial downward penetration of a gas jet into the liquid bath. The jet penetration at startup is not representative of the classical bubble shape that assumes spherical growth behaviour. The buoyancy of the growing bubble is noticeable by $t=0.18$ s, where the bubble rises and grows along the outer wall of the lance. A liquid jet is seen penetrating up the centre of the lance. The first bubble detaches by $t=0.26$ s and fragments into two rising bubbles that are initially in close proximity to the lance. The simulation shows these first bubbles are not rising in contact with the outer lance wall and further fragments to form smaller bubbles. The initial penetration of the gas jet in the simulation is 45.5 mm.

The simulation predicts that between $t=0.38$ – 0.46 s, the gas has risen near the free surface of the bath liquid creating a broad centralised spout. The spout liquid subsequently collapses and breaks up at a free surface location near the outer vessel wall in the time interval $t=0.50$ – 0.58 s. This results in splash being formed. In the actual case, 3D instabilities will result in the splash being directed in specific directions rather than axisymmetrically. Nevertheless, the axisymmetric simulation provide an averaged splash amount that can still provide visual similarities with the real case and help elucidate the mechanisms that result in splash formation.

For the top-submerged gas injection simulation to proceed for the required period shown in Fig. 8, the numerical

code must be robust, so that the simulation can model many bubble detachments. The displayed simulation frames at $t=0.91$, 1.14 and 1.24 s show that, even after many bubbles have disengaged at the free surface and despite the chaotic bath flow, the simulation is still able to generate interfacial profiles that are realistic. The $t=0.91$ s simulation frame shows that the simulation models the ejection of splash drops well clear of the bath free surface. The ability of the simulation to resolve the ejections of splash droplets far away from the lance is very encouraging as it demonstrates that the fine scale phenomena near the outer vessel wall can be resolved even with an axisymmetric numerical model.

6. Conclusion

A numerical code based on the VOF method, capable of simulating the fluid flow of multiple fluids for metallurgical applications, was developed. The use of a multigrid GMRES solver has enabled large density ratios up to 30 000 and fine scale interfacial features to be resolved. The rise of air bubbles in water and liquid iron was studied. The code showed that air bubbles larger than 3 mm rise with substantial shape deformation and the rise velocity varies with the instantaneous shape. For bubbles that do not break up, the periodic variation in velocity was found give an average velocity that agreed with experimental correlations of bubble velocities. For a bubble larger than 12 mm, the code predicted that the bubble was unstable and broke up on ris-

ing in water, but was stable when rising in liquid pig iron. Surface tension was found to stabilise the bubble during rise. The code is capable of resolving the break up of liquid drops in the simulation of splash formation from a top submerged gas injected lance. Such simulations are of importance in the development of new bath smelting processes where splashing plays a major role in either limiting or promoting the process.

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