MATHEMATICAL MODELING OF METALLURGICAL PROCESSES

Stein Tore JOHANSEN

SINTEF Materials Technology

Department of Flow Technology

Trondheim , NORWAY

http://www.sintef.no

Email: Stein.T.Johansen@sintef.no

ABSTRACT

Mathematical modeling has for a long time been of crucial importance for the understanding and prediction of phenomena in the heavy industries. Previously, the main source of knowledge was practical experience with operations and use of simplified, but fundamental understanding of the chemistry and materials that was involved in the processes. Lately, during the last three decades, the development of the digital computers has offered new tools to the process analyst. Today, Computational Fluid Dynamics (CFD) software is, at least in the larger companies, used on a daily basis in order to support new developments and troubleshoot operational problems. The cornerstone in CFD software is the mixture of physical models and the numerical technologies that are used for solutions of the governing transport equations.

As the number crunching capabilities of the computers expand, the limitations in penetrating the inner depth of the processes seems to be less attributed to the computer power, but rather more to the human capability to describe the physics of the phenomena involved. In particular, the predictive power of the models is clearly linked to the physical understanding on which the models are built. Heading for more complex industrial problems, development of robust and predictive models is expected to be a considerable challenge for the years to come.

The models that are used in describing metallurgical processes range from single-phase turbulent flow models dealing with mixing, ventilation and environmental transport problems. Into the hart of the processes we have the most complex multiphase and multi-physics problems, with complex chemistry. In such cases empirical data is hard to obtain, and the model is the only insight into the process.

Examples of applications of modeling and experimental validation work are given. The applications span over the entire field of process metallurgy, ranging from metal production to melt refining and solidification.

Some expectations to the development of the field during the current decade are presented.

NOMENCLATURE

$\mathbf{B}$	-magnetic flux density vector
g	-gravity
h	-enthalpy
k	-thermal conductivity
k_p	-turbulent energy of phase p
$\mathbf{J}$	-electric current density vector
$\mathbf{J}^*$	-general diffusive flux vector
p	-pressure
S	-generalized source term
Sc_t	-turbulent Schmidt number
t_p	-particle relaxation time
$\mathbf{u}$	-velocity vector
V	-volume
V_k	-phase volume
X	-mass fraction

Greek letters

α	-volume fraction
ρ	-phase density
Φ	-viscous dissipation
$\boldsymbol{\tau}$	-stress tensor
$\nu_{p,t}$	-turbulent kinematic viscosity of phase p
σ	-electric conductivity

Subscripts

p	-particle
k	-phase k
f	-fluid

Other

$\langle \ \rangle^i$	-intrinsic average

INTRODUCTION

Since 1983 the Department of Flow Technology at SINTEF Materials Technology has been involved in Computational Fluid Dynamics (CFD) simulations of metallurgical processes. Already at an early stage it became evident that most metallurgical processes are of a multiphase nature and that different multi-phase techniques must be adapted or developed to meet these challenges. In some cases we have chemical reactions where reaction kinetics play a role. Hence, due to the complexity of the metallurgical systems it is important to have a good understanding of the problem before modeling. This will be the starting point that makes it possible to come up with a computationally tractable model that has relevance.

In this paper we will give a sketch of the model concepts that are used in our research group. We will further give some applications, ranging over the entire range of metallurgical processes, from mineral dressing to solidification and shaping of metals.

Summaries of some of these works are found in Johansen (1997), Johansen (2002A) and Johansen (2002B).

VOLUME AVERAGED FIELD DESCRIPTIONS OF METALLURGICAL PROCESSES

The basic Eulerian equations, describing multiphase systems, are given by the conservation of mass, momentum, energy and species in single-phase systems. These basic equations are the mass conservation:

$$\frac{\partial}{\partial t}\rho + \nabla \cdot (\rho \mathbf{u}) = 0 \qquad (1)$$

The momentum conservation equation:

$$\frac{\partial}{\partial t}(\rho \mathbf{u}) + \nabla \cdot (\rho \mathbf{u}\mathbf{u}) = -\nabla p + \nabla \cdot \boldsymbol{\tau} + \rho \mathbf{g} + \mathbf{J} \times \mathbf{B} \qquad (2)$$

Here we note that equation (2) may also describe solid phases. In this case $-\nabla p + \nabla \cdot \boldsymbol{\tau}$ are the total stresses acting inside the phase. The enthalpy conservation equation is:

$$\frac{\partial}{\partial t}(\rho h) + \nabla \cdot (\rho \mathbf{u} h) = \frac{D}{Dt}p + \nabla(k\nabla T) + \Phi + \frac{\mathbf{J}^2}{\sigma} \qquad (3)$$

and finally the species conservation equation:

$$\frac{\partial}{\partial t}(\rho X_m) + \nabla \cdot (\rho \mathbf{u} X_m) = \nabla(\rho D_m \nabla X_m) \qquad (4)$$

We could add more conservation equations, conserving electric charge ionic species and so on when necessary. The general form of these equations can be given as:

$$\frac{\partial}{\partial t}(\rho \Theta) + \nabla \cdot (\rho \mathbf{u} \Theta) = \nabla \cdot \mathbf{J}^* + S \qquad (5)$$

The equations above give a good description of the local transport within each phase, provided that all transport coefficients, the thermodynamic relations, the electric current and magnetic flux density are known. However, in most metallurgical systems we have complex flows with a large number of coexisting phases and components. By employing volume averaging of properties and field quantities (Slattery, 1967; Whitaker, 1967; Grey and Lee, 1977), we may use the basic transport equations as a starting point to derive macroscopic equations that are computationally tractable and that can be used in simulations of metallurgical processes.

The volume average of some property Θ, belonging to a phase indexed k, is defined on a control volume V, where the phase k occupies a volume V_k:

$$\langle \Theta_k \rangle^i \equiv \frac{1}{V_k}\int_{V_k} \Theta_k dV = \frac{V}{V_k}\frac{1}{V}\int_{V_k} \Theta_k dV = \alpha_k \langle \Theta_k \rangle \qquad (6)$$

The volume-averaged velocities are then defined based on mass averages:

$$\langle \mathbf{u}_k \rangle^i = \frac{\langle \rho_k \mathbf{u}_k \rangle^i}{\langle \rho_k \rangle^i} \qquad (7)$$

Here α_k is the volume fraction and $\langle \Theta_k \rangle$ is the volumetric average of Θ_k on the control volume. A detailed procedure for deriving macroscopic transport equations is found in Meland and Johansen (2003). Using the integral form proposed by Prosperetti and Jones (1984) we arrive at the general form for the volume averaged generic equation (5):

$$\frac{\partial}{\partial t}(\alpha_k \rho_k \Theta_k) + \nabla \cdot (\alpha_k \rho_k \mathbf{u}_k \Theta_k) = \qquad (8)$$

$$\nabla \cdot (\alpha_k \mathbf{J}_k) + \alpha_k S_k + \frac{1}{V}\int_{A_k} \mathbf{J}_k \cdot \mathbf{n}_k dS$$

$$-\nabla \cdot \frac{1}{V}\int_V (\alpha_k \rho_k \mathbf{u}_k^{"}\Theta_k^{"})dV - \frac{1}{V}\int_{A_k}\rho_k \Theta_k (\mathbf{u}_k - \mathbf{u}_I) \cdot \mathbf{n}_k dS$$

Here A_k is the bounding surface of phase k inside V, $\mathbf{n}_k$ is the surface normal vector pointing out of phase k and $\mathbf{u}_I$ is the velocity of the interface. The interface velocity and the phase velocity at the interface are identical if there is no mass transfer between the phases. We may note that mass transfer is here caused by either mass transfer or phase transitions such as melting, solidification, vaporization and condensation. Now we introduced the volume averaged fields in the first three terms (brackets removed), while in the three last terms we are still dealing with local quantities. The fourth term that contains terms $\Theta_k^{"} \equiv \Theta_k - \langle \Theta \rangle_k$ comes from the volume integral on the left-hand side of equation (5). This term is often incorrectly omitted, as discussed by Shyy et al. (1997). The phase interaction terms are represented by F:

$$F = \frac{1}{V}\int_{A_k}\mathbf{J}_k^* \cdot \mathbf{n}_k dS - \frac{1}{V}\int_{A_k}\rho_k \Theta_k (\mathbf{u}_k - \mathbf{u}_I)\cdot \mathbf{n}_k dS \qquad (9)$$

The first term in equation (9) represents diffusion type of fluxes to the interface between phases. In the momentum equation (2) this term represents all phase interaction such as drag, global pressure gradient effects, lift and added mass. In the enthalpy equation (3) this term represents the heat exchange between the phases, and in the species equation the term represents diffusion controlled mass exchange between the phases.

The last term in (9) represents the effects of total mass transfer between the phases. This terms accounts for both diffusion and phase transitions. The derivation of this term can be quite lengthy and will necessarily involve a number of modeling assumptions. However, this step is crucial for arriving at useful and consistent models. A basic assumption here is that the mass transfer can be separated in two physical mechanisms. The first mechanism is the diffusional mass transfer that is derived from the diffusional interactions in the species equations, and the second mechanism is phase transition that must be obtained from the full thermal and species balance at the interface. In the latter case, the combined species and thermal conduction to the interface control the mass transfer due to phase transition.

In the derivation of the interfacial transport terms it may be useful to assume that chemical reactions are infinitely fast and that a *local thermodynamic equilibrium* exists at the interfaces between different phases. This will simplify the model, as in most high temperature situations this is a good

approximation. The boundary condition for the temperature and interface compositions can now be computed if the equilibrium thermodynamics is known. This is a beautiful feature of the approach using volume-averaged equations. We realize that thermodynamic equilibrium should in real situations only be applied as locally boundary conditions in a field description. In addition, if the phases contain reactive components, a local thermodynamic equilibrium between phase internal species may be assumed as a reasonable approximation.

The direct application of a global thermodynamic equilibrium, disregarding that the transport processes take place on a large number of time- and length-scales, may lead to very erroneous results.

Multiphase flow simulation using interphase tracking

An alternative Eulerian method to describe multiphase systems is interface tracking (Scardovelli and Zaleski, 1999). This approach is particularly attractive when we are dealing with continuous phases or fully resolve the dispersed phases by the numerical method. In these method markers or color fields (volume fractions) are convected to keep track of interface positions. The method is basically a single-phase method with discontinuities in physical properties. We have developed a Volume-Of-Fluid procedure (Johansen, 1998) to compute separated flows in metallurgical systems. In large-scale engineering applications the species and thermal boundary layers cannot be resolved due to limited computer power, thus limiting the applicability of the method. Overcoming these limitations will be a nice challenge in the years to come.

Lagrangian methods for dispersed phases

In some cases it is favorable to use the Lagrangian formulation for descriptions of particles, droplets or bubbles. The Lagrangian conservation equations for the mass of a particle is:

$$\frac{d}{dt} m = \Gamma \tag{10}$$

where Γ is that transfer rate of mass to the particle from other phases. This term is closely linked to the second term in (9), when $\Theta = 1$. The momentum is conserved by:

$$\frac{d}{dt} (m\mathbf{V}) = m\mathbf{g} + \mathbf{f}_{fluid} + \mathbf{J}_p \times \mathbf{B}_p V_p + \mathbf{f}_{mass\ transfer} \tag{11}$$

In equation (11) $\mathbf{f}_{fluid}$ denotes the forces caused by interactions with the surrounding fluid. $\mathbf{J}_p \times \mathbf{B}_p V_p$ is the Lorentz force acting on the particle, and where $\mathbf{J}_p$ is the average current density through the particle, $\mathbf{B}_p$ is the particle average magnetic flux density and V_p is the particle volume. The last term $\mathbf{f}_{mass\ transfer}$ denotes the momentum supplied to the particle due to mass transfer and phase transition. The enthalpy of the particle is conserved by:

$$\frac{d}{dt} (mh) = \dot{Q}_{fluid} + \frac{\mathbf{J}_p^2}{\sigma_p} V_p + \dot{Q}_{mass\ transfer} \tag{12}$$

Here $\dot{Q}_{fluid}$ is the heat transfer due to thermal conduction, $\frac{\mathbf{J}_p^2}{\sigma_p} V_p$ is Ohmic heating and $\dot{Q}_{mass\ transfer}$ is the enthalpy transfer rate due to mass transfer. In the case of phase transition $\dot{Q}_{fluid}$ will not depend directly on the external temperature but rather on the interface temperature that is controlled by the phase diagram for the local thermodynamic equilibrium.

In order to compute the particle velocities we need to relate the particle position $\mathbf{x}$ to velocity:

$$\frac{d\mathbf{x}}{dt} = \mathbf{V} \tag{13}$$

By using the "Particle Source in Cell" concept, as described by Crowe et al. (1977), we may account for the two-way coupling between particles and the continuous fluid. The interaction between dispersed Lagrangian particles and continuous fluid can also be accounted for directly in transient simulations. The effects of different forces acting on particles and bubbles, including turbulence effects, have been discussed in previous works (Johansen, 1990). The Lagrangian treatment of particles can be extended to deal with particle-particle interactions by the so-called Discrete Element Method (DEM) (Johansen and Laux, 1999).

Turbulent flows

Most real flows are turbulent. Accounting for turbulence effects is hence crucial. By ensemble averaging the volume averaged equations (equation (8)) we may arrive at turbulent flow transport equations. Ensemble mass averaged velocities $\tilde{\mathbf{u}}_k$ are now defined by:

$$\langle \alpha_k \mathbf{u}_k \rangle \equiv \langle \alpha_k \rangle \tilde{\mathbf{u}}_k \tag{14}$$

and we have defined mass averaged fluctuations $\mathbf{u}_k \equiv \tilde{\mathbf{u}}_k + \mathbf{u}_k^{''}$ which has the property:

$$\langle \alpha_k \mathbf{u}_k^{''} \rangle \equiv 0 \tag{15}$$

Based on these definitions turbulent dispersion effects will not appear in the mass continuity equations and the dispersion mechanism will reappear in the momentum equations (Meland and Johansen, 2003).

Typically, the volume and ensemble averaged momentum equation for dispersed particles will look like:

$$\rho_p \frac{\partial}{\partial t}\left(\alpha_p \tilde{\mathbf{u}}_p\right) + \rho_p \nabla \cdot \left(\alpha_p \tilde{\mathbf{u}}_p \tilde{\mathbf{u}}_p\right) =$$

$$-\alpha_p \nabla p + \alpha_p \nabla \cdot \tilde{\boldsymbol{\tau}}_f + \alpha_p \rho_p \mathbf{g}$$

$$+ \frac{\alpha_p \rho_p}{t_p}\left(\tilde{\mathbf{u}}_f - \tilde{\mathbf{u}}_p\right) - \frac{\rho_p \nu_t}{t_p Sc_{tp}}\frac{\nabla \alpha_p}{1 - \alpha_p} \qquad (16)$$

$$-\rho_p \nabla \cdot \left(\alpha_p \overline{\mathbf{u}_p'' \mathbf{u}_p''}\right)$$

Here only drag force is accounted for and electromagnetic forces are neglected. The drag force is linearized and the relaxation time depends on the particle Reynolds number. The gradient term in volume fraction is a result of the ensemble averaged drag term and accounts for the turbulent dispersion effects (Meland and Johansen, 2003). Finally, we have the Reynolds stress term that due to the Boussinesq approximation can be modeled as:

$$\overline{\mathbf{u}_p'' \mathbf{u}_p''} = \frac{2}{3}k_p \mathbf{I} - \nu_{p,t}\left(\nabla \tilde{\mathbf{u}}_p + \left(\nabla \tilde{\mathbf{u}}_p\right)^T\right) \qquad (17)$$

Here, the turbulent kinetic energy k_p of the particle phase can be related to the energy of the carrier fluid, or it can be modeled by its own transport equation. Both ways may be proceeded in a formal manner. The turbulent kinematic viscosity $\nu_{p,t}$ may be modeled from phase internal turbulent energy and dissipation rates, or it may be related to the continuous phase turbulent kinematic viscosity (Johansen, 1990).

At this point we note that accurate predictions of the turbulence field often are the difference between success and failure in predicting flows and processes. The industry standard models are based on the k-ε model (Launder and Spalding, 1974). Presently, the development of transient models necessitates new engineering approaches to turbulence modeling. One of several promising development routes is the hybrid RANS-LES models that combine the strength of RANS models like the k-ε model with the advantageous features of LES models (Johansen et al., 2003).

APPLICATIONS

The multiphase models that have been developed over time have been implemented into various versions of the commercial general purpose CFD-codes supplied by Fluent Inc. Some of the models have been hard-code direct into the source code, while more recently the models have been implemented by User Defined Functions (UDF).

Aluminum reduction cells

The flows in reductions cells, driven by Lorentz forces and anodic release of gas, has been subject to several studies (Johansen, 1997; Johansen 2002A). In more recent work, my colleague K. Bech has improved the models and implemented these into body-fitted grid versions of the FLUENT codes. The models now include effects of anodic gas production (Lagrangian treatment), electromagnetic

fields and specific models for electric surface potential variations (overvoltage) that may effect the electric current distribution and thereby the entire process. In Figure 1 we see predictions of an aluminum reduction cell with vertical electrodes. The gas bubbles produced at the anode are modeled by the Lagrangian method.
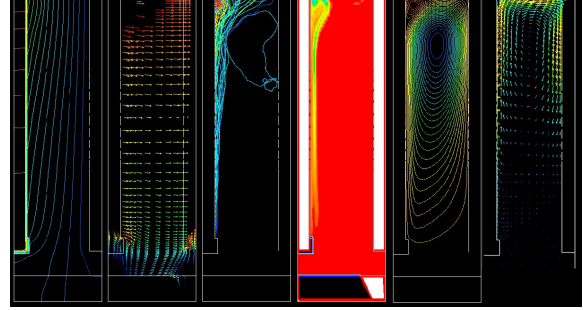

Figure 1 The figure shows a prediction of a reduction cell with vertical electrodes. Calculation of primary and secondary current distribution coupled with bath and gas flow. From left to right we find: Iso-potential lines, Electric current vectors, Bubble tracks, Electrical conductivity, Bath stream lines and Bath velocity vectors (Bech et al., 2001).

In Figure 2 we see a simulation of a bipolar $AlCl_3$ cell. A small inclination of the electrodes causes the gas bubbles to move to the left and setting up a large-scale convective flow pattern. Necessary mass transfer and heat transfer phenomena, such as ohmic heating is straight forward to include in the simulations.
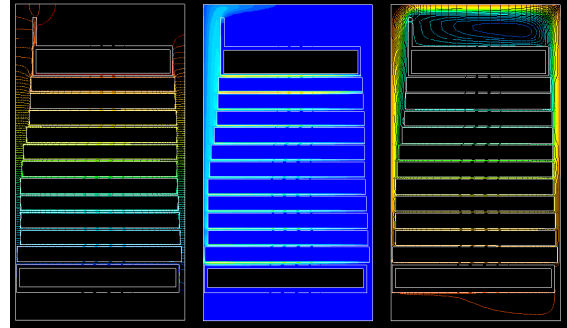

Figure 2 Prediction of Bipolar electrodes Alcoa $AlCl_3$ cell (US patent 4133727, 1979). From left to right we find: Iso-potential lines (0-33 V), Gas volume fraction (mixture model) and Electrolyte circulation (stream function) (Bech et al., 2001).

Ferro-Silicon metal production

In the Ferro-Silicon furnaces the process itself is transient due to the cycles of furnace operations. Hitherto, there has been no attempt to derive full multi-fluid models for the furnace operations. However, this should be within reach using the volume averaging methodology sketched above. The processes taking place below the charge surface are indicated in Figure 3. The flow of raw materials inside the furnace have been analyzed by granular flow multi-field models (Laux, 1998). In Figure 4 we se typical predictions for the flow of gas and solids in such a furnace. The predicted surface shape is in good qualitative agreement with observations.
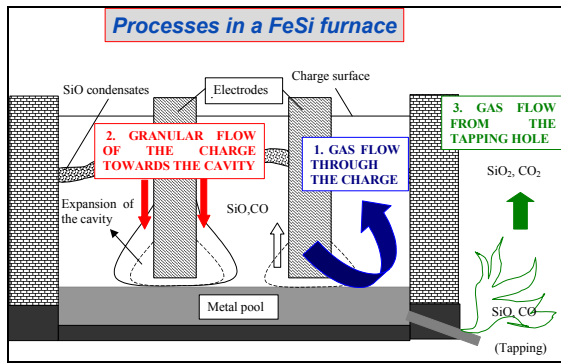
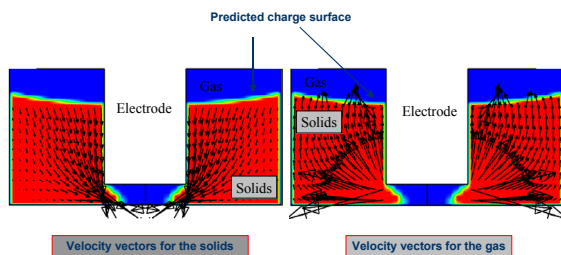**Figure 3** Overview over key processes taking place in a FeSi furnace (Tveit et al., 2002)

Figure 4 The figure shows predicted profiles of process gas and solid charge materials. The computation is cylinder symmetric and represents 1/3 of a typical furnace. Velocity slip is assumed on the electrode in the center.

CFD has been used as a key tool in recent redesigns of off-gas systems at different FeSi plants in Norway. Staff of our Flow Technology Department have analyzed the off-gas combustion, gas collection in the hood, transport and burn-out of soot and charge particles, carbon loss, heat transfer and particle deposition on channel walls. A typical simulation is depicted in Figure 5, where the furnace hood is removed. We see the three electrodes, the charging pipes, the furnace body and two off gas channels that merge into the smokestack and then branch off into a horizontal channel. The furnace port in the foreground is open while the two side ports are closed. The colored surface represents the interface of the flames and the colors represent flame temperature. This type of studies must be accompanied by fast industrial measurements of local temperatures, gas composition, particle concentration and particle composition (Johansen et al., 1991).

Figure 5 Predicted gas flow in off-gas system at Furnace 1 at Elkem Thamshavn, Norway.

Nitrous oxides are formed when process gases combust (Ravary and Johansen, 1999). Here CFD has proven to be a valuable tool to assess operating conditions, as well as the qualitative effects of different process parameters.

Tapping and metal refining

During tapping of steel, effective mixing and effective dissolution of alloying elements are of great importance. Here CFD has proven invaluable for assessing effects of falling jet height, metal depth, effects of alloy density, size and shape (Berg et al., 1999). One particular problem that was highlighted was that gas entrained by the liquid metal jet could effect the flow pattern significantly. No direct experimental information was available. However, thermocam pictures revealed that the industrial tapping jet was quite rough. Then, the gas entrainment was studied by 2D VOF simulations (Johansen, 1998) and combined with existing empirical expressions for gas entrainment in plunging water jets. These entrained gas flow-rate was than fed into a two fluid Eulerian simulation of the combined gas bubble and steel flow. The bubble size was predicted by a transport model for the average size (Laux & Johansen, 1999). The resulting flow is seen in Figure 6. The colors denote the predicted bubble size and the

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contours are streamlines. The flow is downward in the center of the jet. However, due to the buoyancy of the entrained gas bubbles the flow turns direction close to the surface and moves in the opposite direction in the slag layer at the top. The bubbles are small but numerous in the high dissipation shear layer at the rim of the plunging jet. In the quiet zones of the steel the bubbles coalesce and separate from the melt as they reach the surface. These simulations indicate that only full multi-field calculations are capable to explain tapping flow phenomena (Laux et al,, 2001).
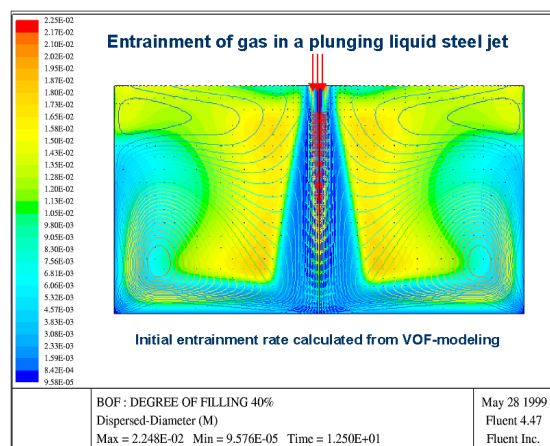

Figure 6 The distribution of area mean bubble size and flow field (streamlines) during tapping of steel (Laux et al., 1999).

In metal refining a combination of CFD and experimental techniques has been a corner stone for improved understanding and process improvement. In Figure 7 we see that slag or large bouyant particles become re-entrained into the melt if the turbulent flow velocity exceed certain limits in mean and rms velocity. Such phenomena can be simulated (Johansen et al, 2003) and the phenomena can be isolated and quantified.

Another important phenomenon in metal refining is agglomeration of inclusions. Through a close cooperation with S. Taniguchi, Tohoku University, Japan, we have suggested that the combined mechanism of agglomeration and break-up should be considered (Johansen and Taniguchi, 1998). A particle size grouping method has been proposed (Nakaoka et al., 2001) that makes it possible to solve multi-fluid problems, solving only for a limited number of size classes. In this work the combined fluid and particle flow with a size spectrum containing 10 particle size classes was analyzed.

Inclusion removal by flotation can be analyzed by both Eulerian-Eulerian or Eulerian-Lagrangian methods. We analyzed combined fluid flow and inclusion removal (Hop et al., 1996), and found that the latter method offers a very versatile way to analyze the removal efficiencies in the case of a "frozen" bubble size distribution. However, a crucial input to such a model is the effective inclusion deposition rate to a bubble in a given flow situation. Such local phenomena can be analyzed by detailed CFD and even effects of turbulence on the flotation rate may be analyzed (Johansen et al, 1995; Gammelsæter et al., 1997; Bech and Johansen, 1999). Lagrangian techniques are also well suited to study removal of dissolved gases, such as hydrogen degassing by argon in aluminum (Johansen et al., 1998).
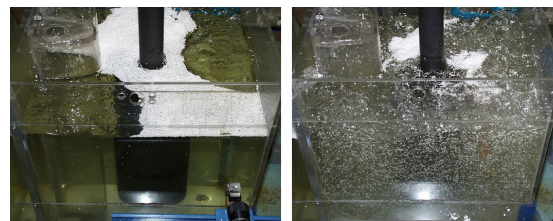

Figure 7 Entrainment of surface slag studied in a rotor-stirred water model of an aluminum-refining unit. The slag (expanded polystyrene particles) is not entrained at low rotor speed (500 RPM, left). At 900 RPM almost all slag is entrained (right).

Metal casting

Some casting phenomena deal with surface tension phenomena and interface dynamics. One example is the study of metal granulation into water, where the complex break-up and solidification phenomena interact. In Figure 8 we see isothermal simulations of metal jet break-up (Johansen, 2002A). By resorting to full 3D simulations information about the granule size distribution may be obtained.
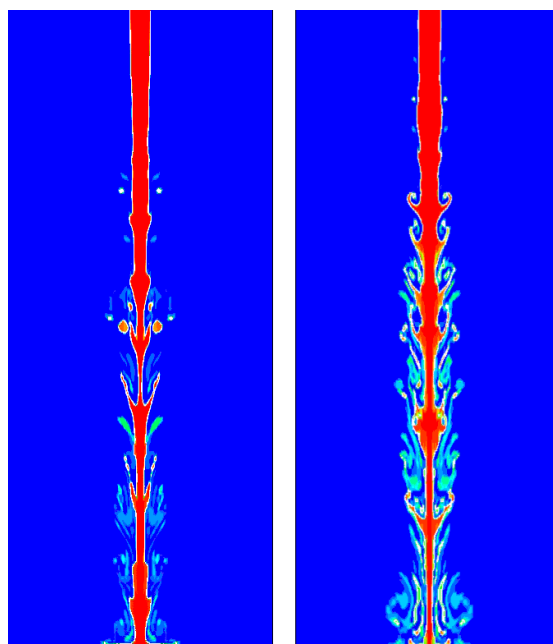

Figure 8 Snapshots of cylinder-symmetrical isothermal predictions of the shape of a jet of liquid metal plunging into water. The initial jet diameter is 16 mm, and the length of the vessel is 500 mm. To the left: Initial velocity is 1.0 m/s. To the right: Initial jet velocity is 4.0 m/s (Johansen, 2002).

Multi-field CFD simulations of casting and solidification phenomena offer very efficient tools to analyze complex phenomena such as macro-segregation (Nilsen et al., 2002). One example is represented by Figure 9 (Laux at al., 2002), where thermal and compositional gradients control the flow and gravitational deposition of crystals on the solidification front have large impact on the macroscopic structure.
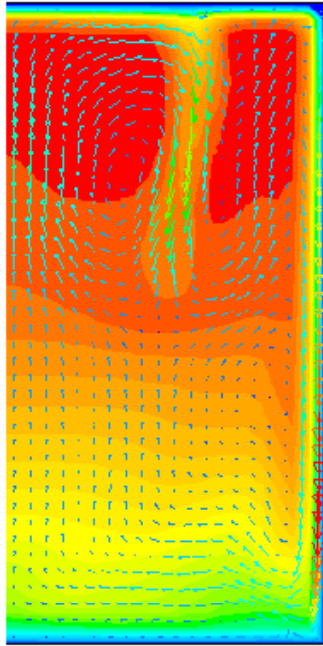
Figure 9 Temperature field and liquid phase velocity vectors from a simulation of solidification of a 30% NH4CL-water solution. The left boundary is isothermal while remaining boundaries are cooled.

CONCLUSIONS

Computational Fluid Dynamics of multiphase systems has emerged as a major tool for understanding and optimizing metallurgical processes, and a number of examples and applications have been given.

Still, both the physical model descriptions and the numerical algorithms have large room for improvements.

Many systems that today are simulated by routine calculations, were only 10 years ago regarded as impossible to model. At the same time new models will be developed for systems that are very complex and that many people today will refuse to accept is possible to model with a required industrial accuracy.

Even the generic modeling concepts will change in the years to come.

Today, relatively complex systems may be described with an acceptable accuracy. Even if the quantitative results are not quite accurate, the relative effects predicted by CFD methods have an astonishing certainty.

One corner stone for multiphase models of metallurgical flows will be the full integration of thermo-dynamics and Computational Fluid Dynamics. Some guidelines for how this can be done, assuming local thermo-dynamical equilibrium, were given above. However, there is significant work to do in this area and access to accurate thermo-dynamical data is prerequisite. Such integrated multi-field thermo-dynamical and flow calculations are expected to create a leap in technology that may have great impact on the industrial development. This will further unify the sciences of flow (kinetics) and equilibrium thermodynamics.

Finally, the predictive power of multiphase CFD in metallurgical systems will rely on new and improved high quality experimental methods to validate models. This is of crucial importance when we deal with high temperature systems with extremely complex physics and chemistry.

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