Mathematical model of inclusion removal during steel degassing

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MATHEMATICAL MODEL OF INCLUSION REMOVAL DURING STEEL DEGASSING

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Abstract

The control of inclusion elimination is getting more and more important to obtain clean steel. This paper presents a methodology under development for predicting cluster growth and elimination in ladle - RH system. The first key point is to express the collision efficiency, which is very specific for alumina cluster due to the non-wetting fluid. Second, a description of the two-phase flow in the system is necessary. In our calculations with Fluent CFD package and Lagrangian approach for bubbles, bubble growth is implemented, which improves the predictions. Using global reactor decomposition makes possible the prediction of the time evolution of cluster distribution. Important effect of fractal dimension is demonstrated.

Introduction

Elaboration of new steel grades requires not only to have a high purity in terms of C, O and N content but also to eliminate particles such as alumina or slag droplets. Flow optimisation making easier inclusion elimination is then a key figure to satisfy cleanliness requirements. Mathematical models of flow and inclusion behaviour are widely used for this purpose (1, 2). But having a predictive tool is still a challenge, because the number of phases is important in steelmaking industry : liquid steel, slag layer, bubbles and inclusions (with a large range of composition and rheology). The paper presents the methodology which is developed at IRSID to predict oxygen content evolution during RH degassing.
The main mechanisms which have to be considered are :
→inclusion growth by turbulent aggregation of elementary inclusions (keeping in mind that liquid steel is a non-wetting medium for inclusions); the difficulty is to express collision efficiency for alumina particles,
→inclusion removal by flotation; the difficulty for alumina clusters stems from the complex morphology of particle; fortunately, the use of fractal concept makes it possible to cope with this problem.
The paper describes the general modelling of inclusion removal taking into account the previous mechanisms. Hydrodynamic parameters are obtained by means of Fluent CFD package and a specific coding is developed for cluster growth.

Modelling

Aggregation
When particles are immersed in a turbulent flow, they are submitted to collisions and, for some of them to aggregation. This mechanism leads to the growth of cluster, which can be considered as the addition of many elementary particles with the same radius a (see Figure 1), in consequence of the successive collisions.

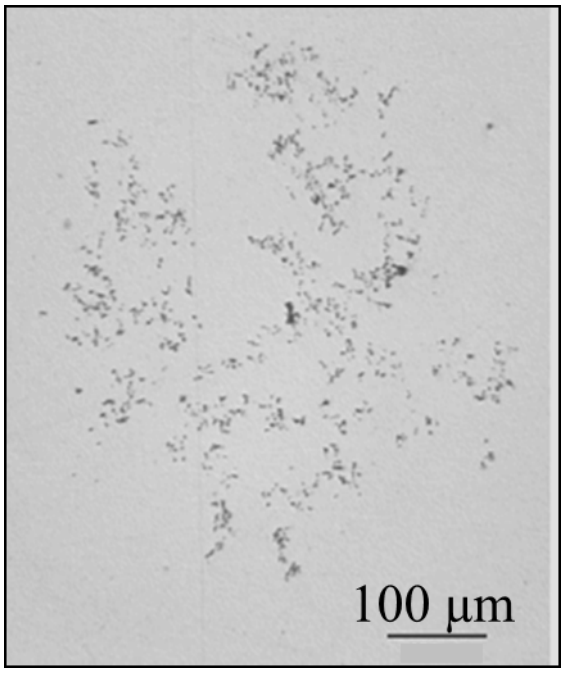


Figure 1 : Typical shape of alumina cluster

The main effect of non-wetting conditions, associated with alumina and liquid steel, is a possible fluid slippage on the solid surface, generally characterised by the distance b, Figure 2 :

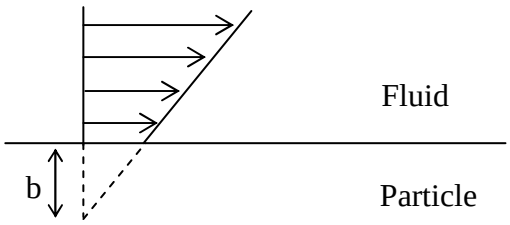


Figure 2 : fluid behaviour for hydrophobic surface

This was already observed by some authors over lyophobic solid surface system (3) and there are many evidences that a gas layer between hydrophobic particles can be created (4, 5, 6, 7), which is probably one of the main reasons for the slippage. The modelling of the hydrophobic interaction was already proposed by authors, which took into account not only the collision rate, but also the efficiency for collisions to produce aggregation (6). Expression obtained for collision efficiency is :

$$\alpha = \left[24 \int_{\delta}^{\infty} \frac{e^{18\pi C_A \frac{1+\frac{3b}{a}}{1+\frac{2b}{a}} F(r')}}{r'^4 G_h(r')} dr' \right]^{-1}$$

where : $\delta = 2 + \frac{h_{\min}}{a}$ and $F(r') = \int_{\infty}^{r'} \frac{1}{s^2} \frac{dV'(s)}{ds} ds$

with r'=r/a V'=6V/A (A : Hamaker constant for particle / fluid / particle system).

The Van der Waals potential is expressed by : V = -A f_{geom} where f_{geom} is a geometry dependant space function.

G_h is a correction function for hydrodynamic interactions when particles are closed to each other (6).

To take into account a possible gas layer covering the inclusion, the lower bound of the integrals is modified with h_{min}. C_A is a non-dimensional parameter comparing attractive Van der

Waals forces to fluid friction. Expression of flow number $Fl=1/C_A$ is given by Kusters et al.(8) in case of cluster contact instead of spherical particles.

The evolution of cluster size distribution in a reactor is simulated by solving a population-balance equation :

$$\frac{dN_i}{dt} = \frac{1}{2}\sum_{j=1,i-1} K_{i,i-j} N_j N_{i-j} - \sum_{k=1,\infty} K_{i,k} N_i N_k - \frac{1}{2}\sum_{j=1,i-1} B_{i,j} N_i + \sum_{j>i} B_{j,i} N_{ji} - F_i$$

This equation, called Smoluchowski equation (9), describes the time evolution of the volume density of aggregate with size i, N_i, and is expressed in terms of aggregation kernel $K_{i,j}$ and fragmentation kernel $B_{i,j}$. It also includes a term F_i for inclusions elimination by flotation or rising effect of fluid flow, using, for large particles, cluster terminal velocity calculation.
In case of particles smaller than Kolmogorov micro-scale, K_{ij} may be expressed by (10) :

$$K_{ij} = \frac{4}{3}\left(\frac{3\pi}{10}\right)^{1/2}\left(\frac{\varepsilon_m}{\nu}\right)^{1/2}(a_i + a_j)^3 \alpha_{ij}$$

ε_m : mean value of turbulence dissipation rate.
a_i : outer radius of aggregate of size i (containing i elementary particles), with the meaning of collision radius.

Because mass transfer should happen immediately after inclusion aggregation in liquid steel, making robust inter-particle connection, assumption was made that there is no cluster break up.

Assessment of cluster terminal velocity

Terminal velocity could be a key parameter for inclusion elimination. Because of the complex geometry of the cluster, adaptations for both drag coefficient and equivalent density must be proposed. Making the assumption that cluster can be characterised by a fractal dimension, which seems to be appropriate for alumina (2), and that alumina cluster consists of many elementary particles with the same radius a, Cournil et al. (6) proposed a procedure to evaluate cluster terminal velocity, based on correlations found in the literature. Table I gives an example of fractal dimension influence on both terminal velocity and cluster radius. It illustrates the main effect of this parameter. It is also very probable that terminal velocity has a minor effect on inclusions elimination and that only first phase velocity has to be taken into account for elimination calculation.

Table I Influence of cluster shape - radius of elementary particle : 0.5 µm

Number of particles in cluster	1000		10000		100000	
Fractal dimension	2.9	2	2.9	2	2.9	2
Terminal velocity (m/s)	$2.8\ 10^{-5}$	$8.6\ 10^{-6}$	$1.3\ 10^{-4}$	$2.6\ 10^{-5}$	5.7 10-4	$7.8\ 10^{-5}$
Radius (microns)	5.4	20.1	12.0	63.7	26.5	201

Fluid flow

In the Fluent Lagrangian modelling, dispersion of bubbles due to turbulence in the fluid phase is predicted using a "random walk" model which includes the effect of instantaneous turbulent velocity fluctuations on the bubble trajectories, through the use of stochastic methods (commonly called the "eddy lifetime" model). The momentum transfer between the continuous phase and the dispersed phase is computed by examining the change in momentum of a bubble as it passes through each control volume and is given by :

$$F = \sum_{m=1}^{m=N} \frac{3\mu C_d Re}{\rho_p 4 d_p^2} (v-u)\dot{m}_p \Delta t$$

v : gas velocity
u : liquid velocity
N : number of particle inside the control volume
Re : relative Reynolds number
d_p : bubble diameter
C_d : drag coefficient
$\dot{m}_p$: mass flow rate of bubbles
Δt : time step

When stochastic tracking is performed, the interphase exchange terms are computed for each stochastic trajectory with the particle mass flow rate, $\dot{m}_p$, divided by the number of stochastic tracks computed.

Limitations of Lagrangian modelling

There are several limitations in this Lagrangian modelling. The first concerns the assumption that the second phase is dilute so that the continuity equation ignores the gas volume fraction. This leads to overestimate the liquid flow rate in the snorkel. Having in mind that gas volume fraction is probably around 10% (see expression in(11)), this problem is probably crucial and could lead, in the future, to chose Eulerian approach which, unfortunately, is not yet available in Fluent 5. The second drawback deals with the turbulence. It is well known that there is an additional production of turbulence due to bubbles. This was already mentioned by many authors (12, 13). This production is not implemented in standard Fluent 5. In consequence, in the up-flow snorkel where most of the bubbles are present, ε should be underpredicted.
But Lagrangian procedure remains attractive : it is easy to implement pressure dependent bubble diameters and to change argon injection location without changing the mesh.
As a practical conclusion, starting with Lagrangian is a good choice to make progress but precise results will probably require Eulerian approach.

More information about CFD modelling

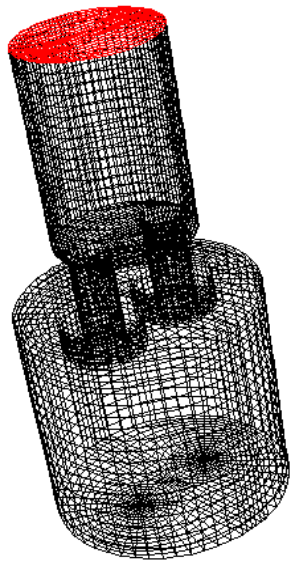


Figure 3 : mesh of RH + ladle reactor

For bubble injection, the diameter is 5 mm and approximately 100 injection points are homogeneously distributed in the section of one snorkel. Each free surface (ladle and RH) corresponds to non-slip condition, with "escape through the boundary" for the bubbles (see Figure 3 for the mesh).
Forces acting on particles that have been considered are : drag force, buoyancy force, virtual mass force and force due to pressure gradient in the fluid. For drag coefficient, the following relation was selected and implemented in Fluent (14) :

$C_D = \frac{0.622}{0.235 + \frac{1}{Eo}}$ which is available for $500 \leq Re \leq 5000$ and $Eo \leq 40$ (ellipsoid or spherical regime).

The argon density, for 1550°C with local pressure corresponding to ferrostatic pressure and vacuum pressure of 500 Pa, is 0.29 kg/m^3 at injection points. Vertical evolution of both bubble radius and density is represented on Figure 4. There is a clear increase of bubble radius, meaning that the mass of liquid steel flowing in the bubble wake is constantly increasing. This should have a positive effect on liquid steel circulation rate.

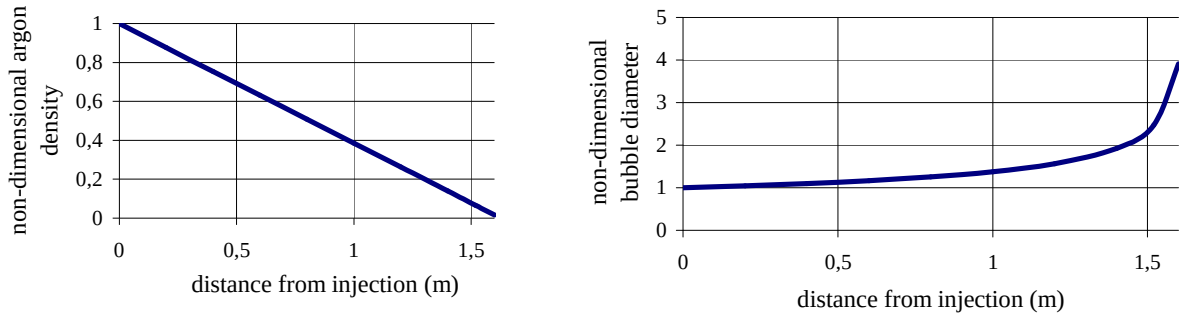


Figure 4 : Dependence of bubble properties on vertical position.

Global modelling

Because it is not possible to follow each inclusion trajectory in a CFD code, taking into account collision and aggregation, a simplified approach was developed. The methodology we chose consists in splitting the reactors in different elementary reactors, each of them characterised by two hydrodynamic parameters :

1. Dissipation rate ε of turbulent kinetic energy,
2. Rising velocity of clusters towards the free surface.

Those parameters are obtained by means Fluent package and defined "inputs" for solving the population balance equation in reactors. The splitting is performed by considering that the turbulence dissipation rate must have the same order of magnitude in each reactor. In our case, 5 elementary reactors were selected.

Validation

It is clear that only a limited number of validations has been performed. The first step deals with a comparison with Higashitani's results (15), who made an extensive study for turbulent agglomeration in a stirred reactor with hydrophilic particles. We compared our calculations to those obtained by Higashitani, with the assumption that all particles are spherical (D_f=3) and efficiency coefficient is fixed to unity. This totally numerical comparison was successful (6). As a matter of fact, there is a clear lack of experimental data for agglomeration with hydrophobic particles. This work is currently under development in a stirred reactor, with silanisation surface treatment of silica particles to get non-wetted surfaces. Validation for this situation, currently under development, will be published later.

The second step concerns the flow in the ladle - RH system. Fortunately, correlations are available, making a link between process parameters. The circulation flow rate is given, for example, by Kuwabara et al. (16) : $Q_m = k.D_i^{4/3}.Q_v^{1/3}$.

D_i : internal snorkel diameter (m) Q_v : argon flow rate (Nm^3.h^{-1}).

Figure 5 summarises the comparisons. The positive point is that Fluent correctly predict the mean velocity in the down-flow snorkel, with the good slope in the curve. If the bubble growth is considered, the velocity is significantly increased with value slightly above those given by the correlation; this is can be explained by the continuity equation which is not properly solved. Further work will be necessary, not only for the continuity equation but also for a better description of argon injection. At this stage, the CFD accuracy is considered to be sufficient to go on the study.

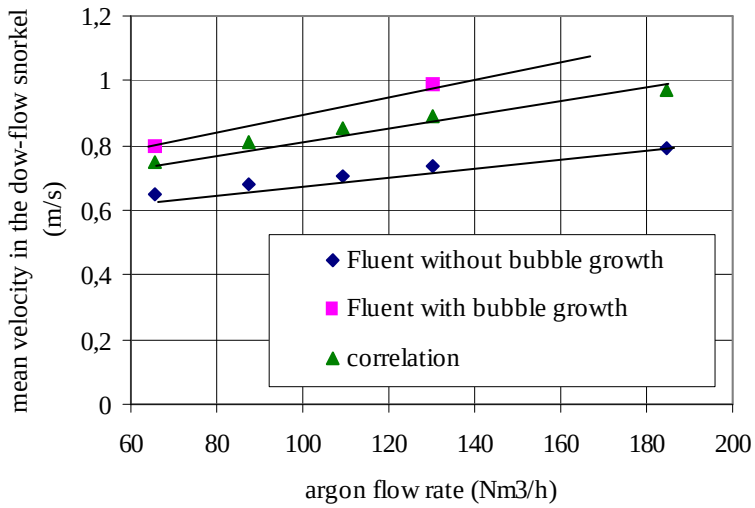


Figure 5 : Comparison of Fluent's results with standard correlation.

Results

The first results concern bubbles at RH free surface (Figure 6). There is a spreading of bubbles along the lateral RH wall when argon flow rate goes up. This phenomenon is exarcebated when bubble growth is included in the modelling (Figure 7), due to the increase of the recirculation rate it produces. It could have been expected that bubbles went out of the domain exclusively above the snorkel. Having a look on the velocity field at RH free surface provides an explanation : when the flow goes out of the snorkel, it flows mainly towards the RH wall and the general movement is from the snorkel to the immediate lateral wall. This is explicit on Figure 9, where laterally injected bubbles are tracked. Bubbles can penetrate deeply in the RH and, if bubble break up occurs, it is probable that small bubbles are pulled in the laddle, promoting inclusion ascent and inclusion elimination.

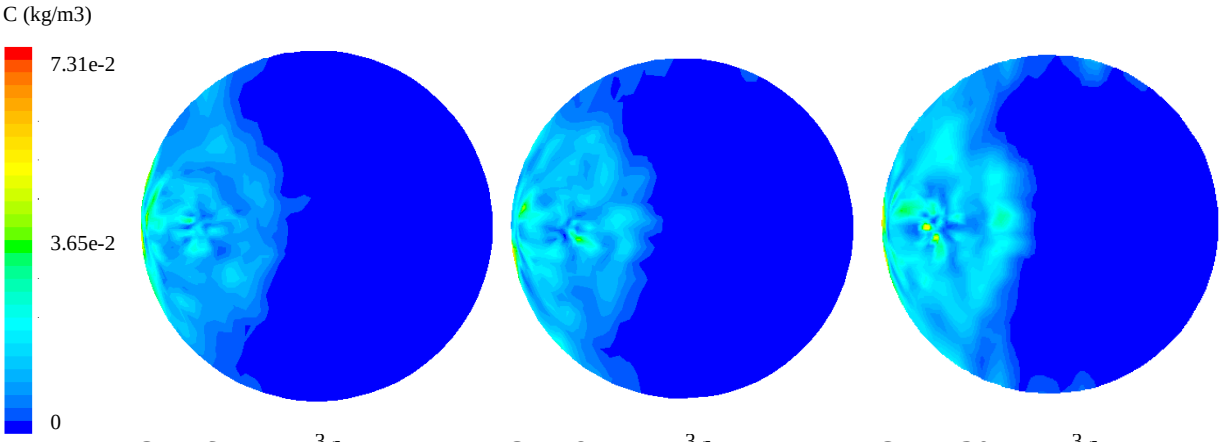


Figure 6 : Bubble concentration at degasser free surface - without bubble growth.

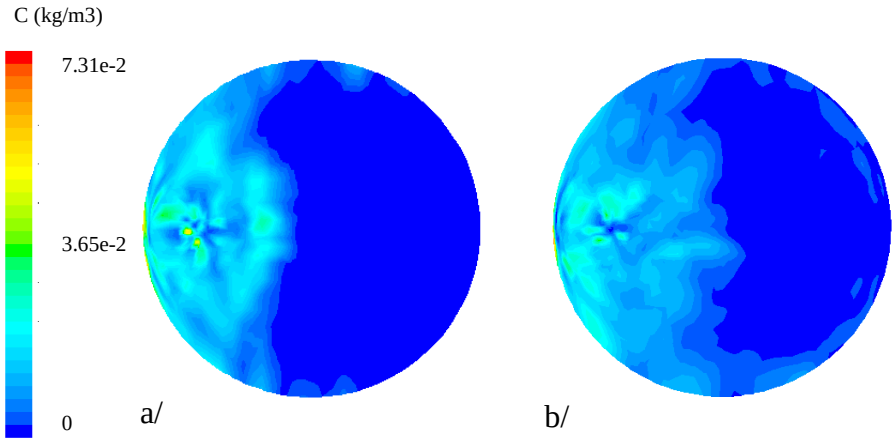
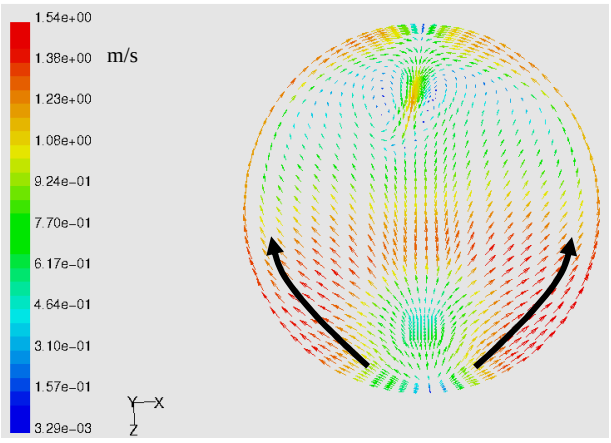
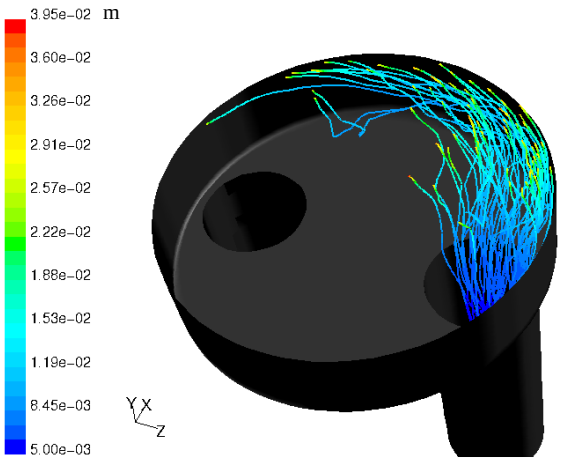


Figure 7: Bubble concentration at RH free surface - a : without bubble growth - b : with bubble growth.



At this stage of our modelling development, effect of bubbles in promoting inclusion elimination is not well understood. They should create turbulence, enhancing agglomeration, that could be taken into account in our model. But bubble bursting should create violent interface disturbances and there is progress to define if this mechanism can affect inclusion agglomeration or fragmentation.

Figure 8 : Velocity field at RH free surface - top view.



The net argon mass flux going in the ladle, even if it is a small fraction of the total injected mass flux, should also be precisely determined, because it could be an efficient way of improving inclusion elimination. This could be evaluated using a critical Weber number, but having good prediction for ε is necessary (17).

Figure 9 : Bubble trajectory, coloured by bubble diameter - Q_g=130.1 Nm^3/h.

There are two parameters which have a major influence on inclusion elimination :
1°/Rising velocity of clusters towards the free surface.
2°/Surface where inclusions are entrapped.

For evaluating the part of the ladle free surface where most of inclusions are entrapped, inclusions were injected in the down-flow snorkel. By examining inclusion concentration near the free surface, it is then possible to evaluate part of the ladle which is active for inclusion elimination. Looking at Figure 10, heterogeneous concentration is observed, proving that the "perfect mixing reactor" approach is not appropriate. It is observed that inclusions are distributed near the lateral wall of the ladle and this region can be considered as the "entrapment active region". The rising velocity is then the mean vertical velocity below surface active region. This basic approach will be improved in the near future, using Residence Time Distribution for different sizes of "frozen" clusters (they do not aggregate). But qualitative analysis is possible with this method which is physically sound.

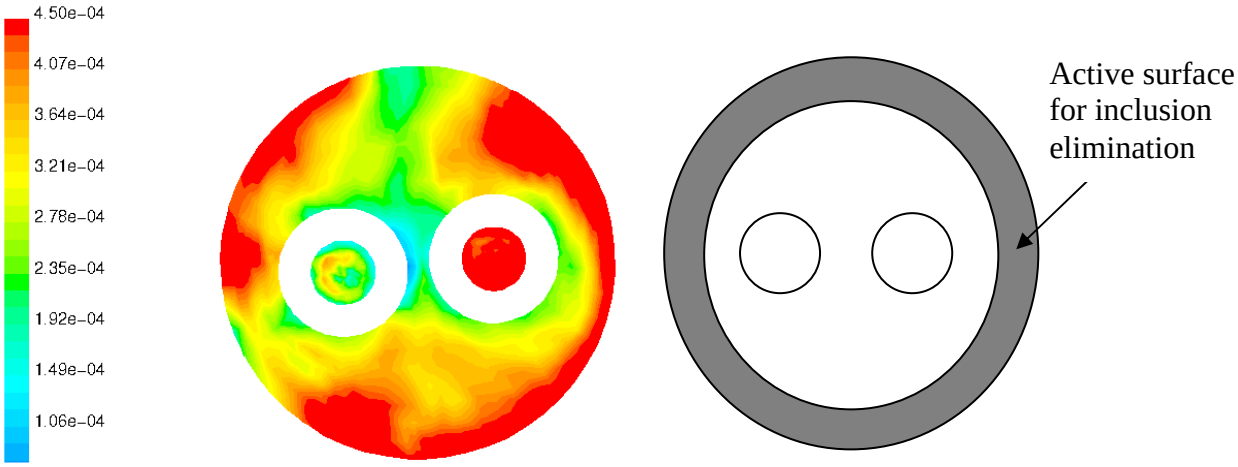


Figure 10 : Inclusion concentration under ladle free surface - Q_g=130.1 Nm^3/h with bubble growth

The previous described models have been applied for initial total oxygen content of 300 ppm. Initial particles are all spherical with 0.5 µm radius. Illustration of influence of fractal dimension is shown in Figure 11. The simulation is limited to cluster with maximum 1024 elementary particles; this explains the peak for D_f=2 and abscissa 1024 which means that a lot

of clusters are larger than 1024. The interesting point is that the assumption of spherical cluster (D_f=3) leads to slow down the appearance of big cluster, compared to D_f=2. This is due to the important collision radius for loose cluster, making easier collisions an growth (see Table I). It is also notable that size distribution is almost linear in semi-logarithmic coordinates.

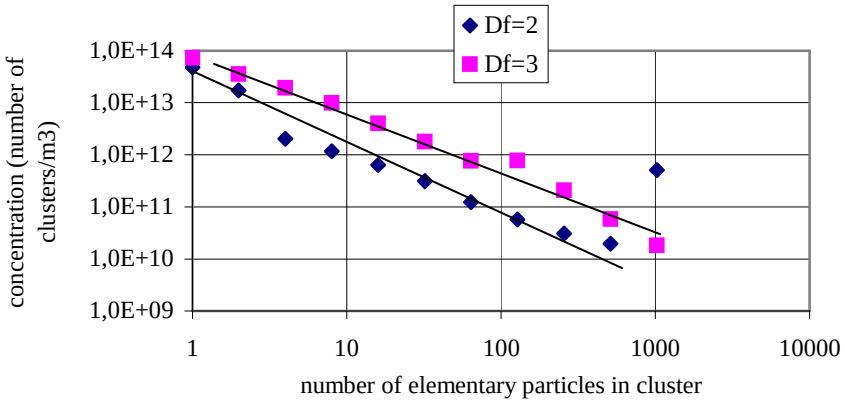


Figure 11 : Influence of fractal dimension (t=100s) - Qg=130.1 Nm3/h - b=10^{-10} m and t=100 s

Calculations of total oxygen evolution were then performed for different argon flow rates : 40 Nm^3/h (metal circulation rate : 70 t/min) and 114 Nm^3/h (100 t/min). As it can be expected, a clear influence of gas flow rate is observed and a linear decrease in semi-logarithmic coordinates appears, which is a common figure for such time evolutions.

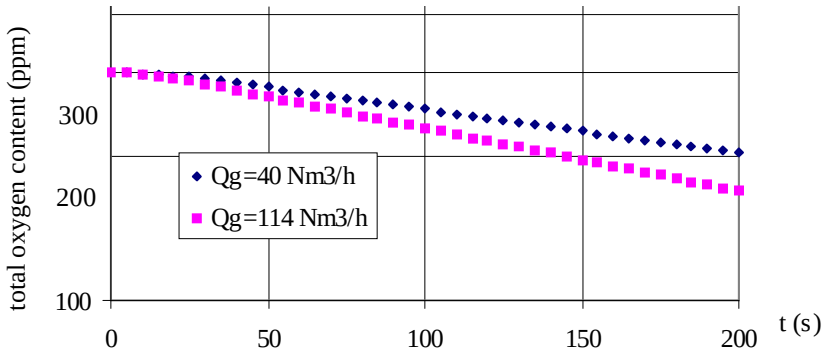


Figure 12 : Time evolution of total oxygen content

Conclusions

This paper deals with the modelling of alumina cluster growth and elimination. This is an attempt to make a link between microscopic phenomena (at Van der Waals force scale) acting on micronic particle and macroscopic scale of a flow in ladle - RH system. Although all the theoretical problems are far to be solved, a methodology is presented here which could be useful for everyone who would like to test its own model.

The main conclusions for the flow analysis in ladle - RH system are :

◊ Because there is an important decrease of the ferrostatic pressure when bubbles go up from injections, it is important to take into account the bubble growth in the snorkel; this lead to a significant increase of the liquid metal recirculation rate and calculations are quite close to standard correlations.

◊ There is an notable spreading of bubbles in the RH; this could lead to pull bubbles in the ladle from the top RH and to promote inclusion elimination.

The cluster shape is characterised by a fractal dimension. Including this parameter is crucial because the growth of loose clusters will be considerably accelerated compared to compact ones. Terminal velocity for loose cluster is quite small compare to compact ones. This means that flotation concept could be inappropriate and that only the first phase movement is responsible for flowing up the clusters.

The modelling for cluster entrapment at free surface is not established and it is not yet possible to distinguish loose cluster entrapment to compact ones. This must refined in the future. Then, comparison with measurements (total oxygen content evolution for instance) will be helpful to adjust the model.

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