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Simulation de phénomènes multi-échelles dans les procédés sidérurgiques

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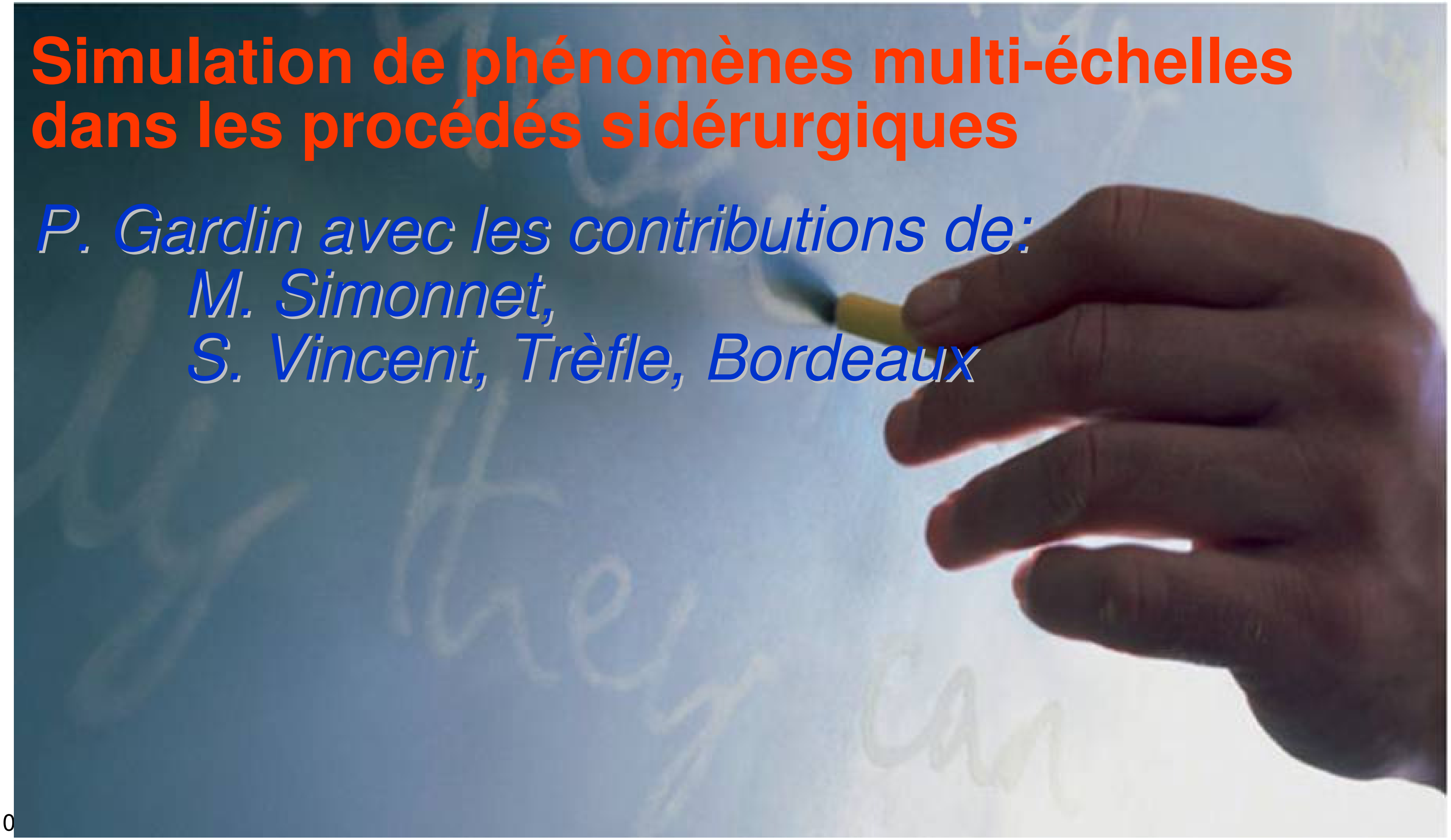
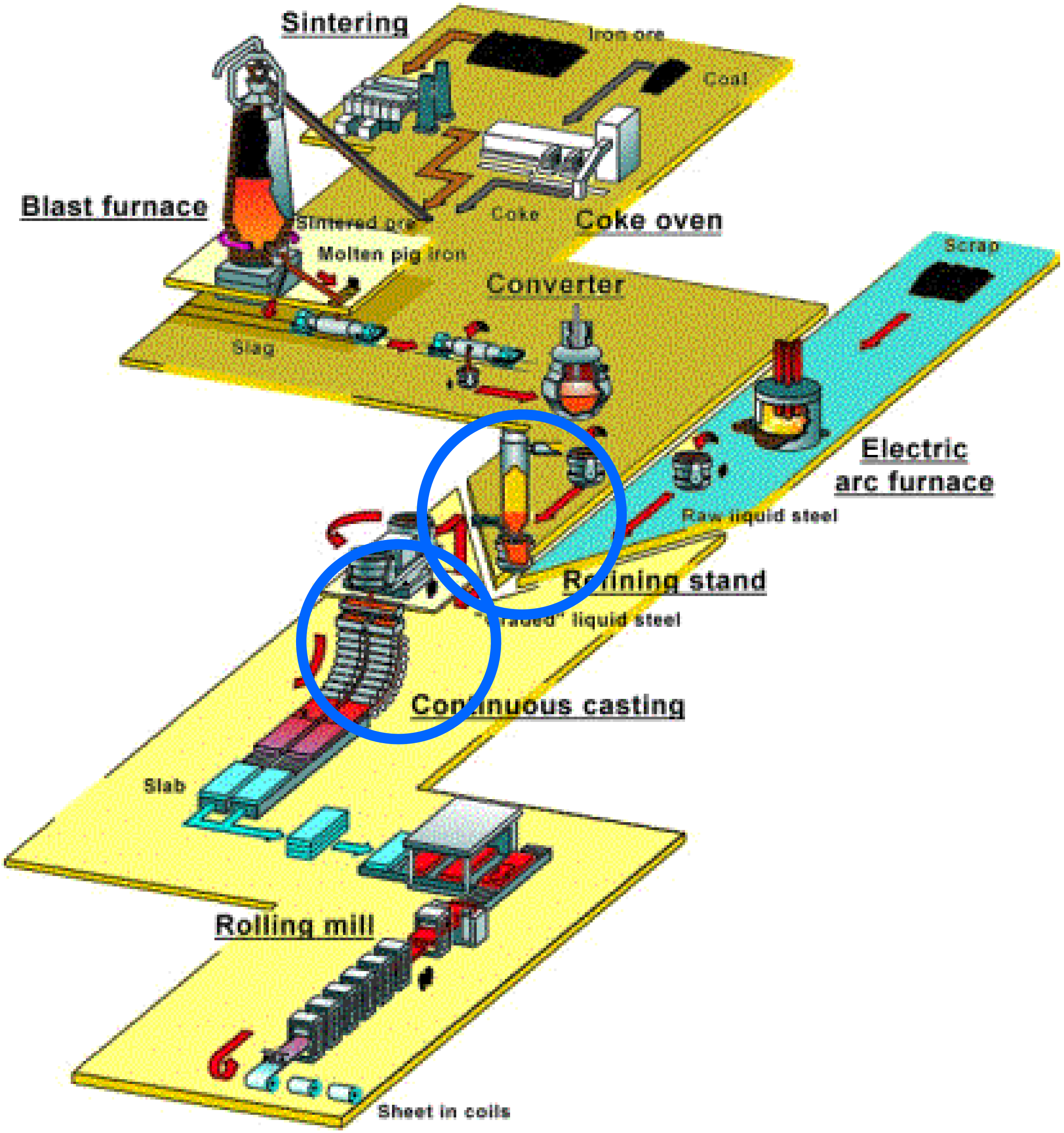


Context

- Different phases are simultaneously present in a steel making reactor: slag, liquid steel, argon, top gas, inclusions (liquid, solid), which can strongly interact (momentum, heat and mass transfer), water/vapour:
  - Experimental facility: good for understanding – scale up: most of the time difficult
  - ***Numerical models***: can deal with industrial process – most of the time: assumptions on mechanisms
- Mechanisms to be studied:
  - a wide range of length scales: from nanometers for nucleation of inclusion in liquid steel to several meters for flow characteristics
  - With mesh: secure method for conservative equations, but cannot considered mechanisms at lower length scale than mesh size
  - Meshless technique: much easier to cope with multiscale problems (lagrangien tracking, lattice Boltzmann, DEM, SPH…), but high cost to deal with the interaction of particles


Sintering
Iron ore
Coal
Blast furnace
Sintered ore
Coke
Coke oven
Molten pig iron
Converter
Slag
Scrap
Electric
arc furnace
Raw liquid steel
Refining stand
"Graded" liquid steel
Continuous casting
Slab
Rolling mill
Sheet in coils

Exemple 1: elimination of inclusion at interfaces

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Decarburation

Decrease H, N, O

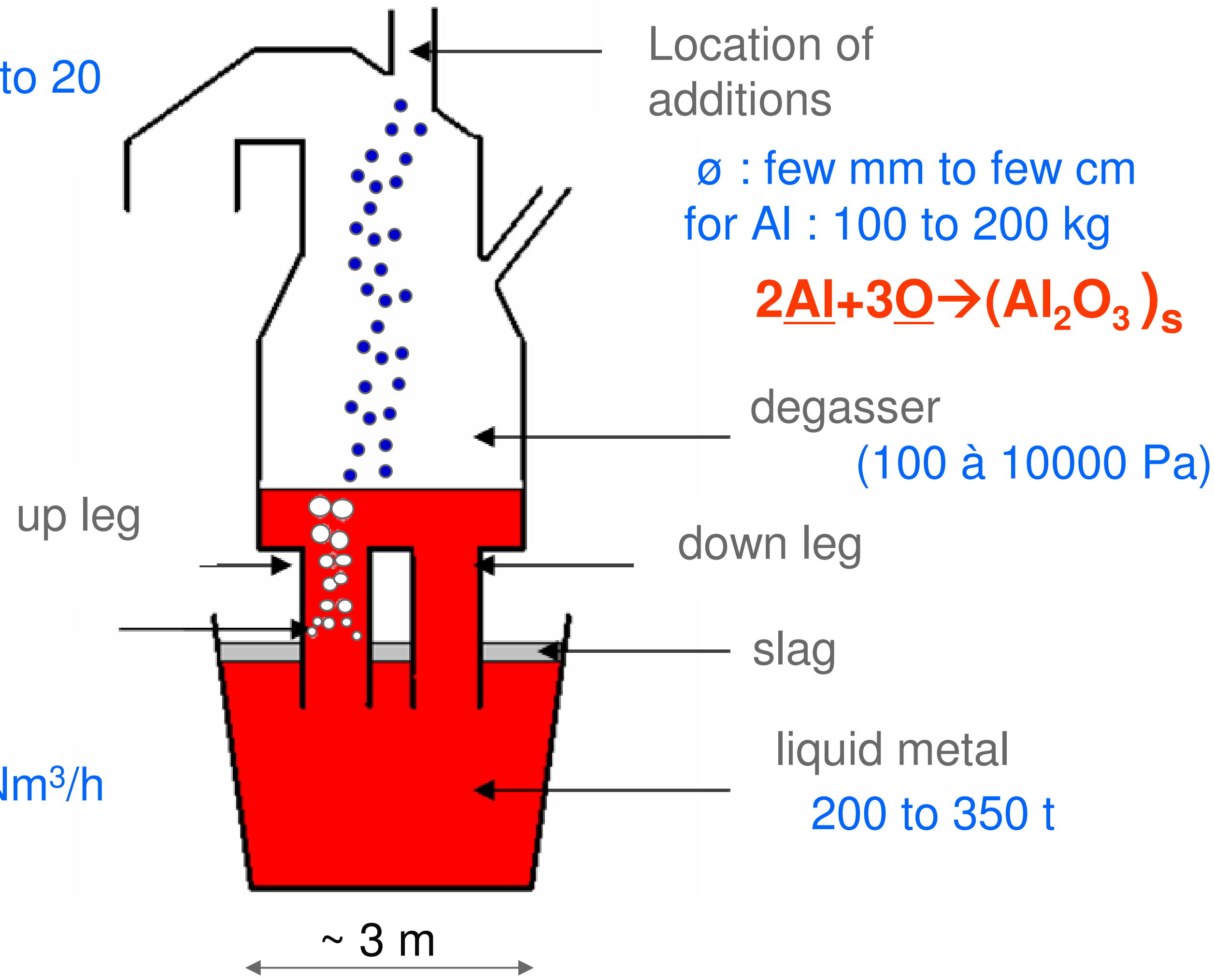
C < 15 ppm after 12 to 20 min vacuum

RH

ladle

Argon gas injection

50 to 150 Nm³/h Ar total



Industrial context

- Metallurgical treatments done in ladle before continuous casting of steel

- Ladle is a reactor where complex multiphase phenomena occur:
  - Steel stirring by argon injection
  - Steel/slag deformation
  - Slag droplets emulsification
  - Solid alloy transport and melting
  - Inclusions precipitation…

- Inclusions control has a crucial role in the quality of continuously cast slabs

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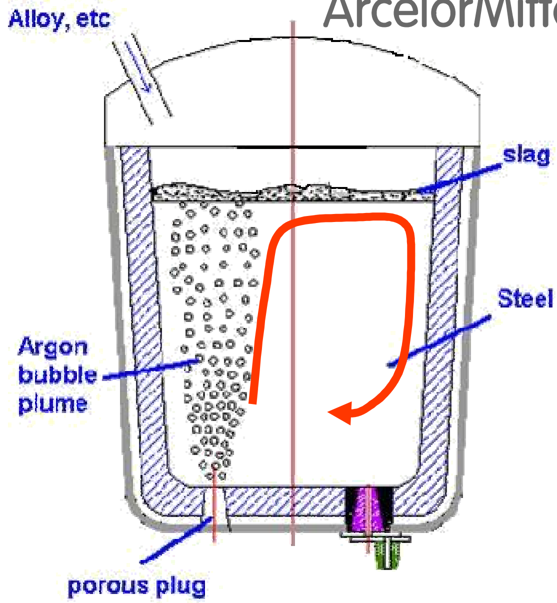

Typical mechanisms to be considered

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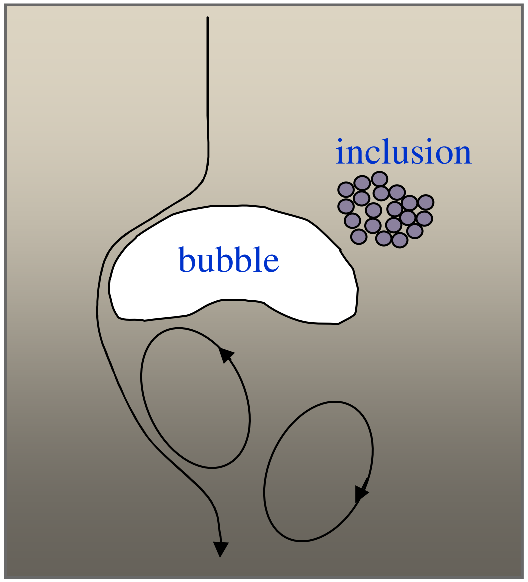
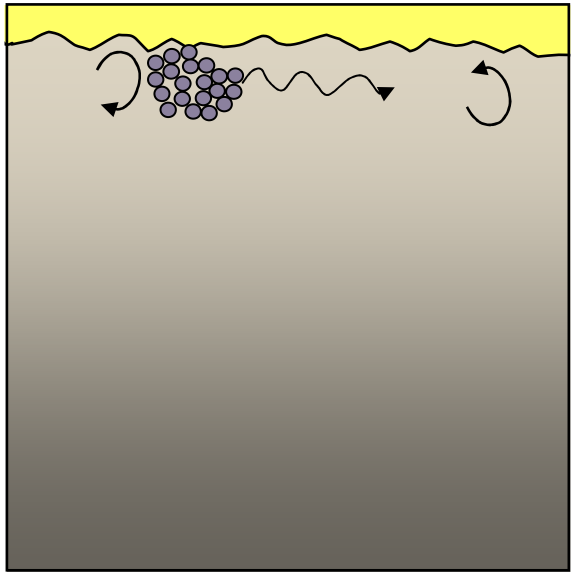
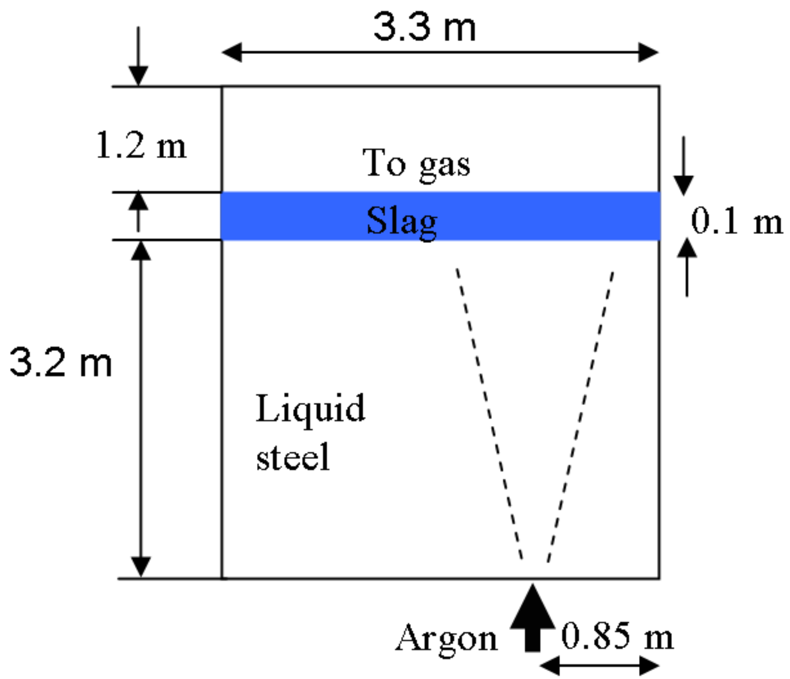




- Particle interaction with interface (gas/liquid/solid)
- Interfacial area, depending on local turbulence and local mass transfer
- Inclusion nucleation/growth/collision/composition
- Bubble break-up, coalescence
- …

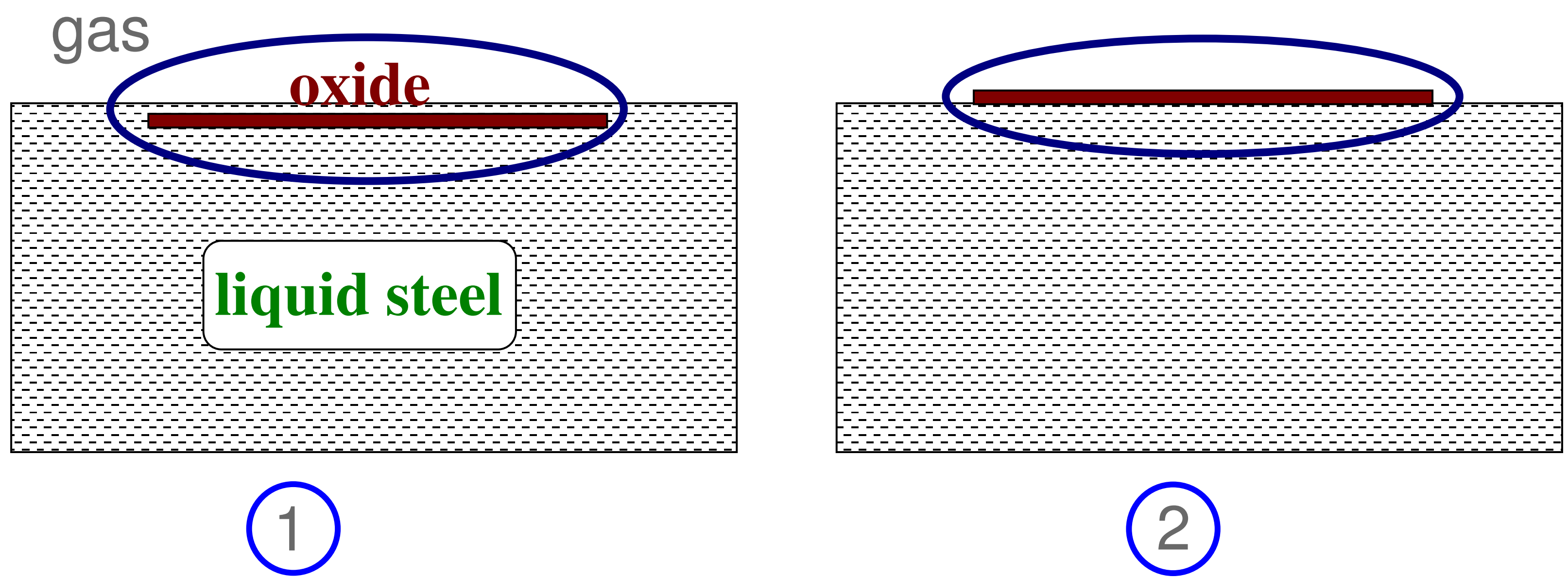
CFD model

- Commercial CFD software AnsysFluent™
- Simulation domain consists of five phases:
  - liquid steel
  - slag layer
  - inclusions
  - argon
  - and upper gas
- Phase interfaces calculated by the VOF method with the Piecewise-Linear Interface Construction (PLIC)
- Inclusions (supposed spherical and solid) trajectories calculated by DPM method.
- In 3D, bubbles are tracked by Discrete Phase Model (DPM) for computational cost reason
- Realizable k-ε turbulence model is used with standard logarithmic wall functions



But correct entrapment criteria of inclusions at interfaces is required

Boundary Condition -Inclusion emersion

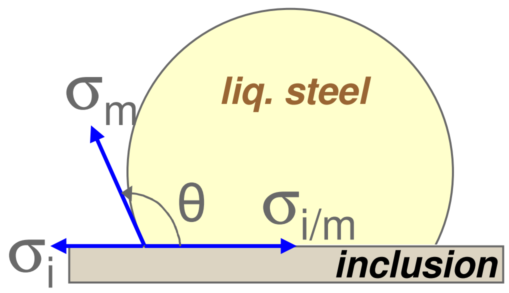


√Spontaneous emersion if free energy for system 2 is lower than free energy for system 1

√Considering that solid oxide piece is small with unit surface and only surface forces can be considered:

$$\left.\begin{array}{l} G_1=\sigma_{i/m} + \sigma_{i/m} + \sigma_m \\ G_2=\sigma_{i/m} + \sigma_i \end{array}\right\} \quad \Delta G=G_2-G_1=\sigma_i - \sigma_{i/m} - \sigma_m$$

BC - Inclusion emersion



√Equilibrium of triple point : $\sigma_i - \sigma_m \cos\theta - \sigma_{i/m} = 0$

$\Delta G = \sigma_m (\cos\theta - 1)$

√Spontaneous emersion if there is a decrease of free energy or $\Delta G < 0$

From Kozakevitch & Lucas, 1971

Inclusion: alumina	θ	σ_m (N/m)	ΔG
Pure iron	140°	1.80	-3.179
Fe, 4% carbon	133°	1.73	-2.910
Fe, 0.07% oxygen	80°	1.10	-0.909
Fe 0.02% sulfur	140°	1.39	-2.455

Dewetting of torical shape film

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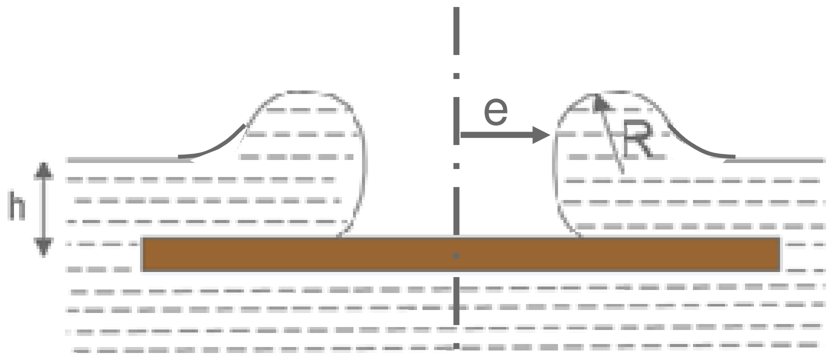
- According to Buguin et al. (1999), in case of dewetting of water on an hydrophobic plate, a toric shape is observed
- We can expect the same behaviour between liquid steel and alumina inclusions

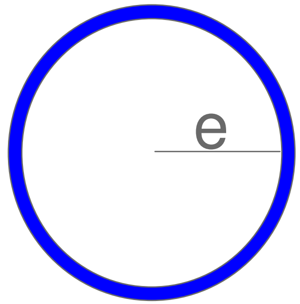
$$\frac{d^2E}{dt^2} = \frac{9}{15E}\left(\frac{dE}{dt}\right)^2 - \frac{2\sqrt{E}}{\rho}\frac{\partial p}{\partial r} - 3\nu\frac{dE}{dt}\frac{1}{h^2}$$

with $E = e^2$



Rim with a toric shape (h=5 µm, θ=110°, σ_m=1.4 N/m, D=200 µm)

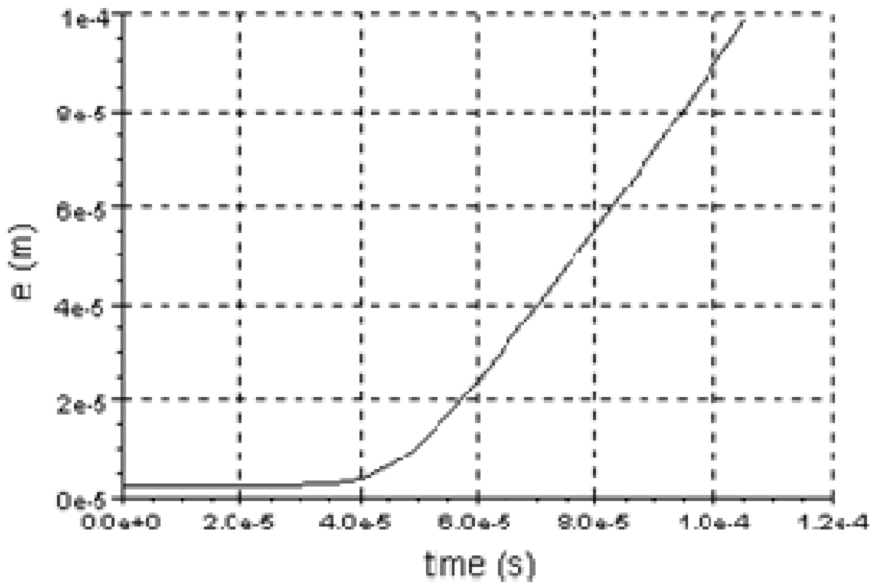
Tore with radius R:



- This 2nd order ODE is solved with Scilab™ software

Withdrawal time compared to turbulence characteristic time

- Evolution of dewetting with constant film thickness (h=5µm, θ=110°, σ_m=1.4 N/m, D=200µm)



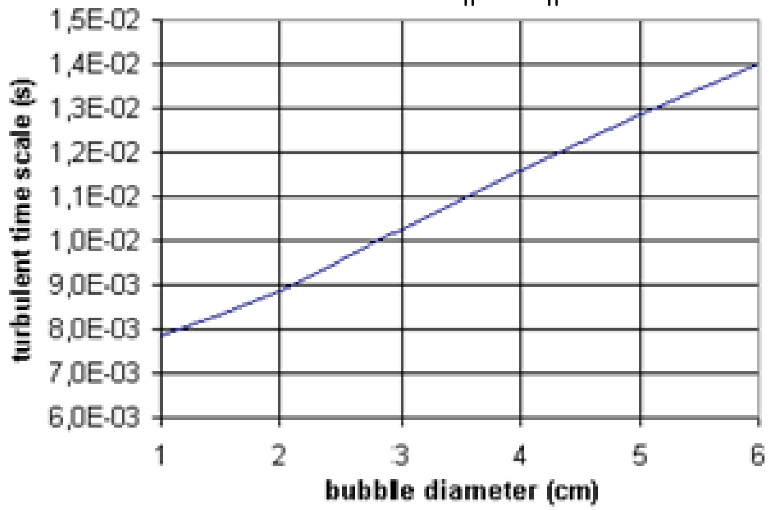
⇨ Film ejection is much more rapid than typical time scales of turbulence

⇨ High entrapment efficiency

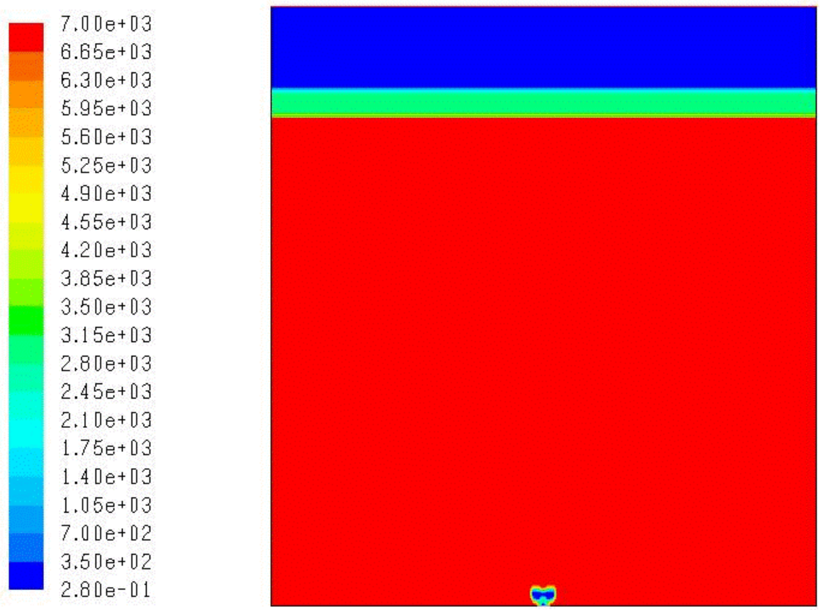
⇨ Robust adhesion, once inclusion is entrapped

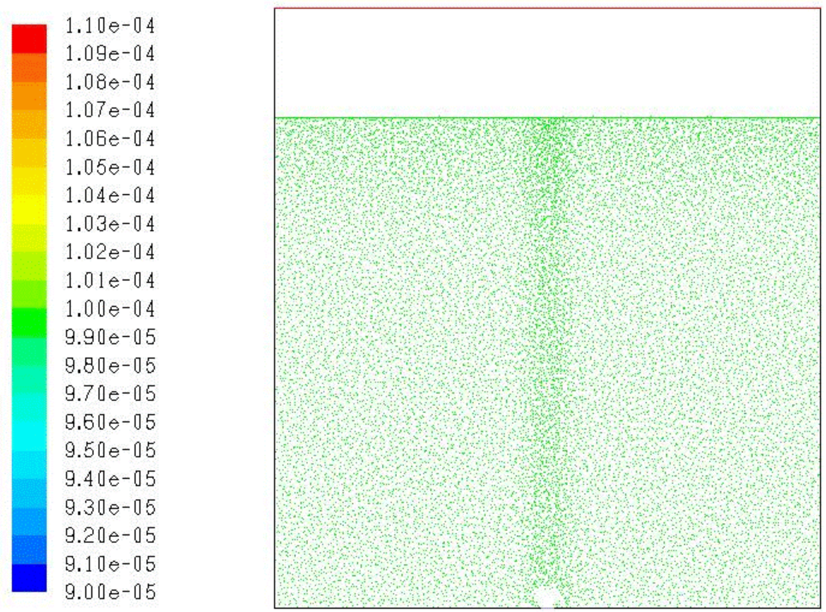
- Bubble Induced Turbulence, due to vortex shedding from the rising bubbles, is the key mechanism for the creation of turbulent eddies in this situation
- Time scale proposed by Lopez de Bertodano (1992):

$$\tau_{turb} = \frac{2C_{VM}\, d_B}{3C_D \left\| \vec{U}_R \right\|}$$



Video of a VOF bubbles 2D simulation

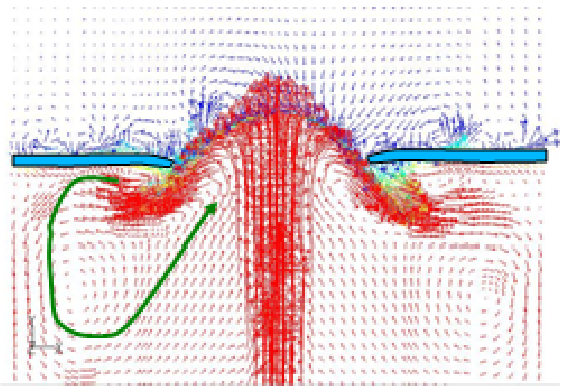


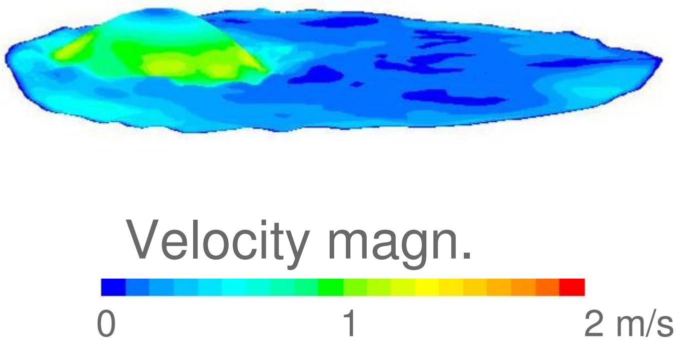


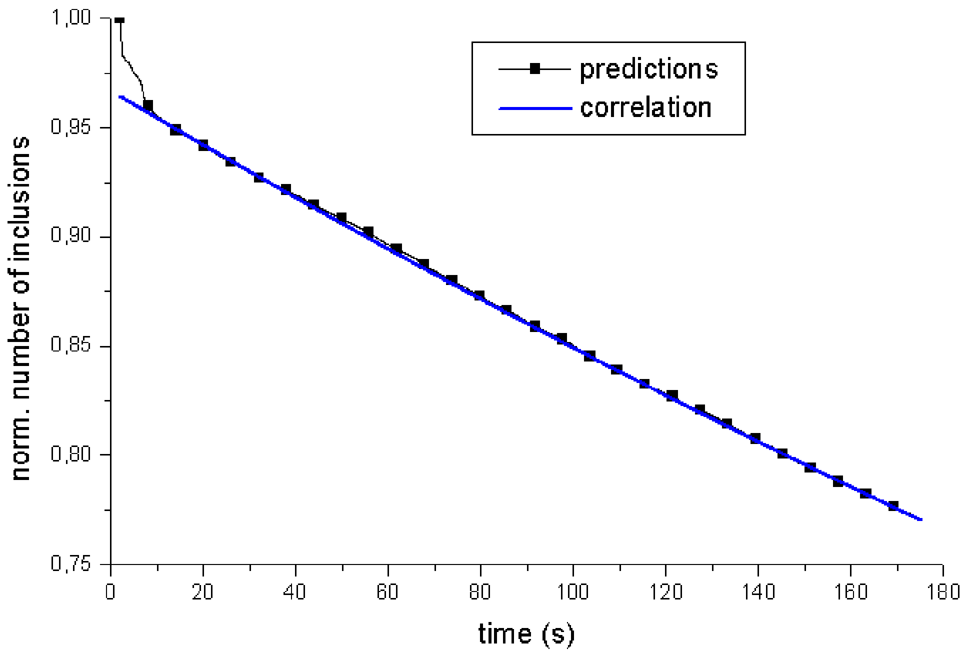
Contours of Density (kg/m3)

Particle tracks ranged by diameter (m)

Time evolution of inclusion number







Stirring power: 35 W/t
τ = 770 s

$$\frac{dC_0}{dt} \propto -\frac{C_0}{\tau}$$

Comparison with experimental results: deoxidation constant

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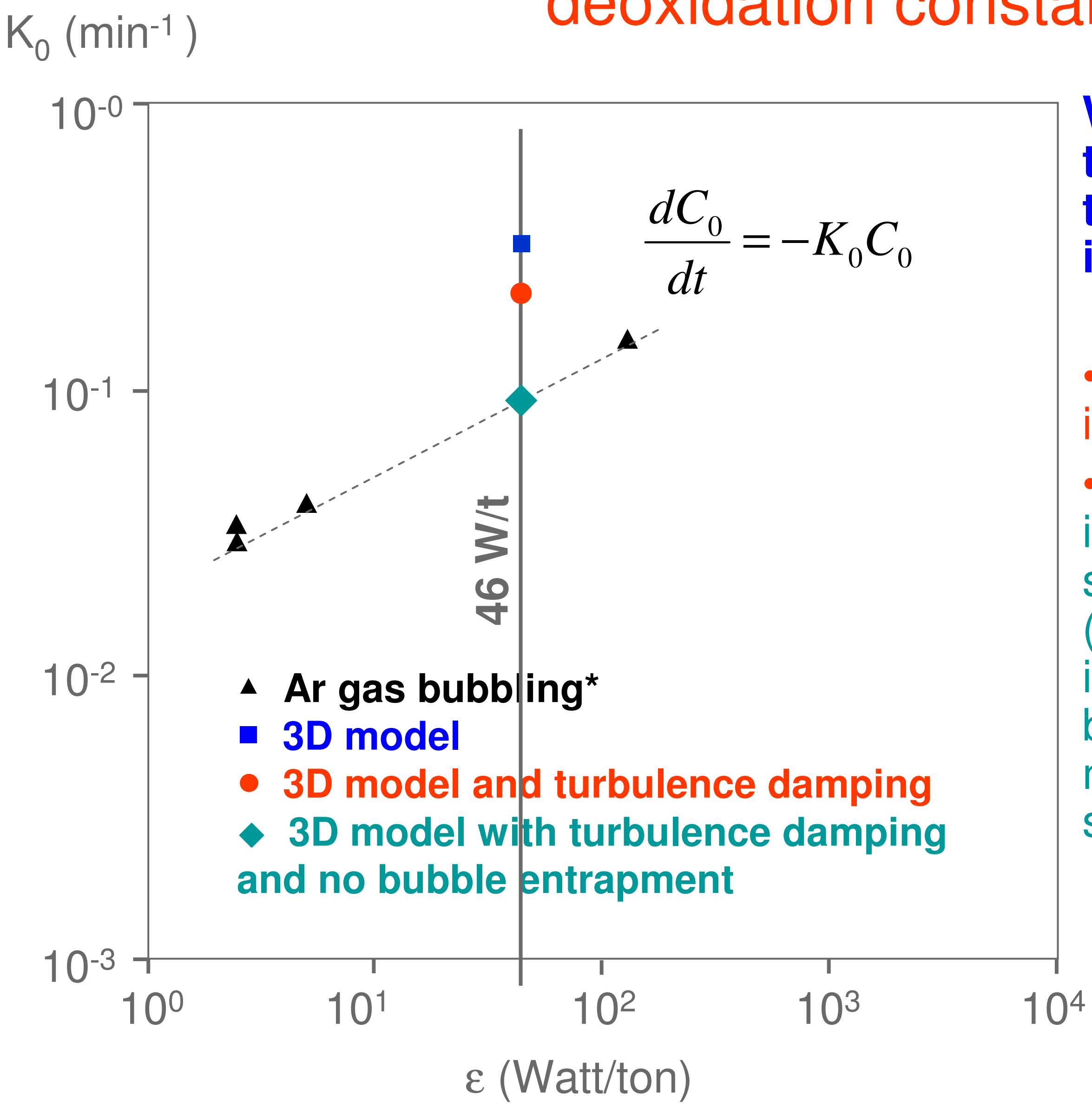


With initial model, we can see that inclusion elimination is too rapid. Possible reasons investigated:

- Turbulence damping at interface should be activated
- Too many interfaces for inclusion entrapment: only liquid steel/slag interface is selected (no entrapment by bubbles, i.e. inclusions are trapped by bubbles but released in molten metal when bubbles cross steel/slag interface)

* industrial data gathered by Zhang and Thomas (2002)

Desulfurization - Industrial context

Decrease of sulfur content in liquid steel.

Basic chemical reaction:

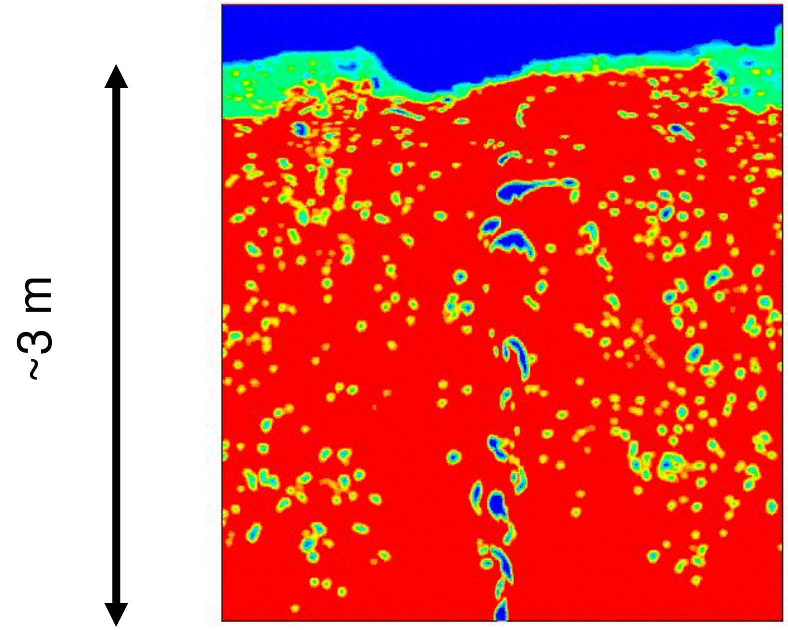
(CaO)+<u>S</u> → (CaS)+<u>O</u>

<u>O</u>, <u>S</u> : dissolved elements in liquid steel

CaO, CaS: lime and calcium sulfide in the s

Kinetics of desulfurization:

$$\frac{d\underline{S}_t}{dt} = -\beta\frac{A}{V}\left[\underline{S}_t - \frac{(S)_t}{L_S}\right]$$



β: mass transfer coeffcient

$\underline{S}_t$, $(S)_t$: sulfur content in liquid steel and slag at time t

A, V: surface of exchange and slag volume

L_s: sulfur partition coefficient between liquid steel and slag

Steel desulfurization

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RFCS report, 2003. Secondary steelmaking:
Desulphurization of liquid steel with refining top slags

Top slag: $\beta_{S,M} = 9.1 \times 10^3 D_{S,M} \sqrt{u_0}$ - metal side

Slag droplet: $\mathrm{Sh} = 2 + \mathrm{Re}^{1/2}\,\mathrm{Sc}^{1/3}$ with $0.5 < \mathrm{Re} < 1000$

$$Sh = \frac{\beta_{S,M} \varnothing_{slag\ droplet}}{D_{S,M}}$$

$$\beta_{S,M} = K\sqrt{D_S \frac{Q}{A}}$$

Riboud-Vasse formalism

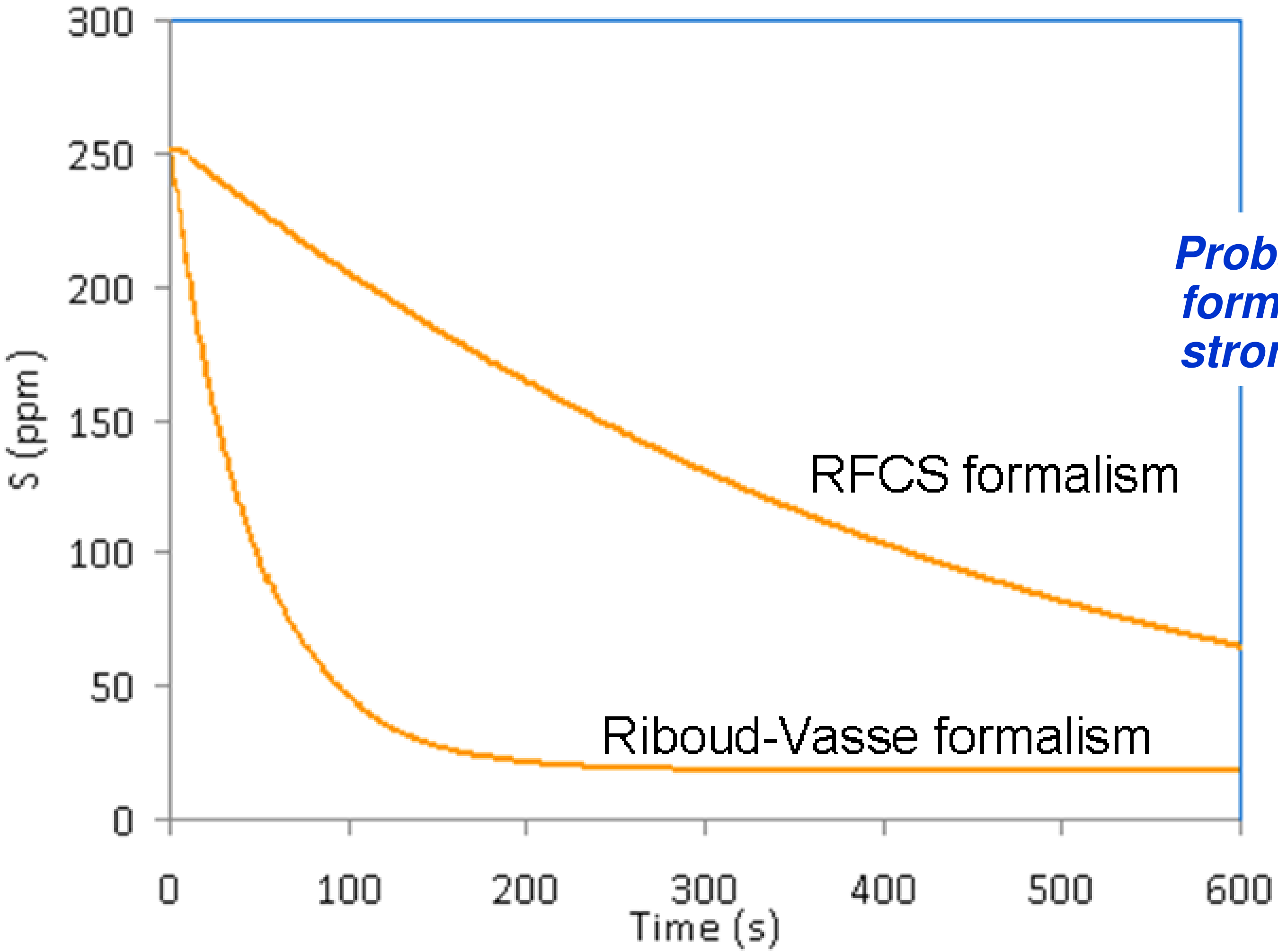
D_S is the sulfur diffusivity in liquid steel

$K \sim 500\ \mathrm{m}^{-1/2}$ - estimated industrially for a wide range of gas flow rate and ladle size

Q: argon flow rate

A: ladle section

Application of the different correlations



Probably: droplet formation from the slag is strongly under predicted

Simpler configuration: continuous casting mold

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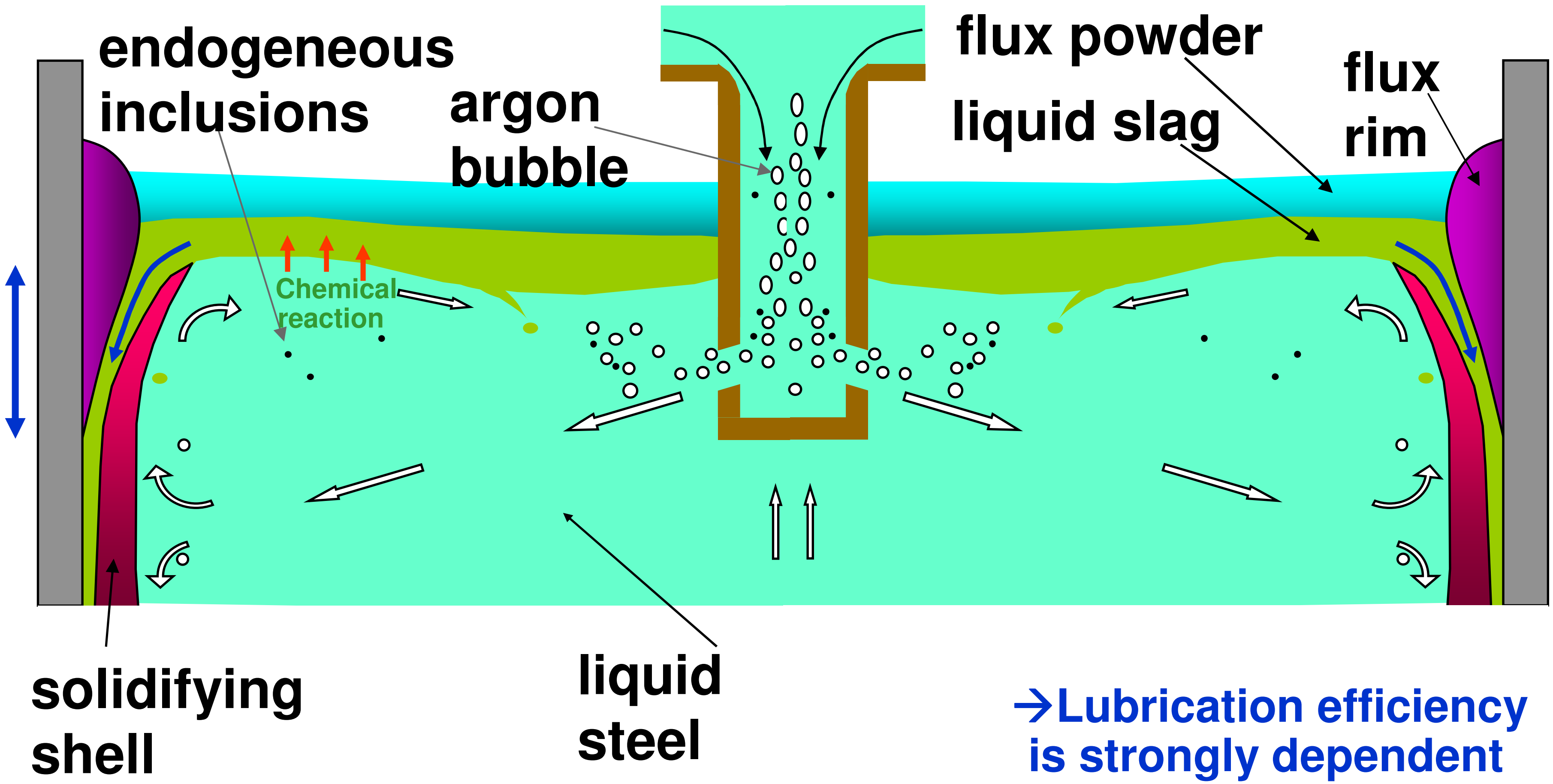

→Lubrication efficiency is strongly dependent on slag viscosity

Calculations with Thetis

→Developed at Institut de Mécanique et d'Ingénierie de Bordeaux – Trèfle Department – specialized for complex interface tracking with turbulence

$$\beta \approx Sc^{-1/2} u^* \mathrm{Re}_t^{-1/2} \left[\left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} \right)^2 \right]_i^{1/4}$$

$div\, \vec{n} = 0$ where $\vec{n}$ is the normal to the interface

(x, y) : interface plane

Surface Divergence Model - BANERJEE, S., LAKEHAL, D., M. FULGOSI, M., (2004), "Surface divergence models for scalar exchange between turbulent streams", *International Journal of Multiphase Flow*, **30**, 963-977.

→The boundary conditions are periodic in the streamwise and spanwise directions

→Symmetry conditions are imposed in the direction normal to the interface.

→Pressure gradient is imposed in the x direction for liquid so that the max velocity in liquid steel is ~0.3 m/s : 5.27 Pa m^{-1}.

→Slag is entrained by liquid steel

Species diffusion

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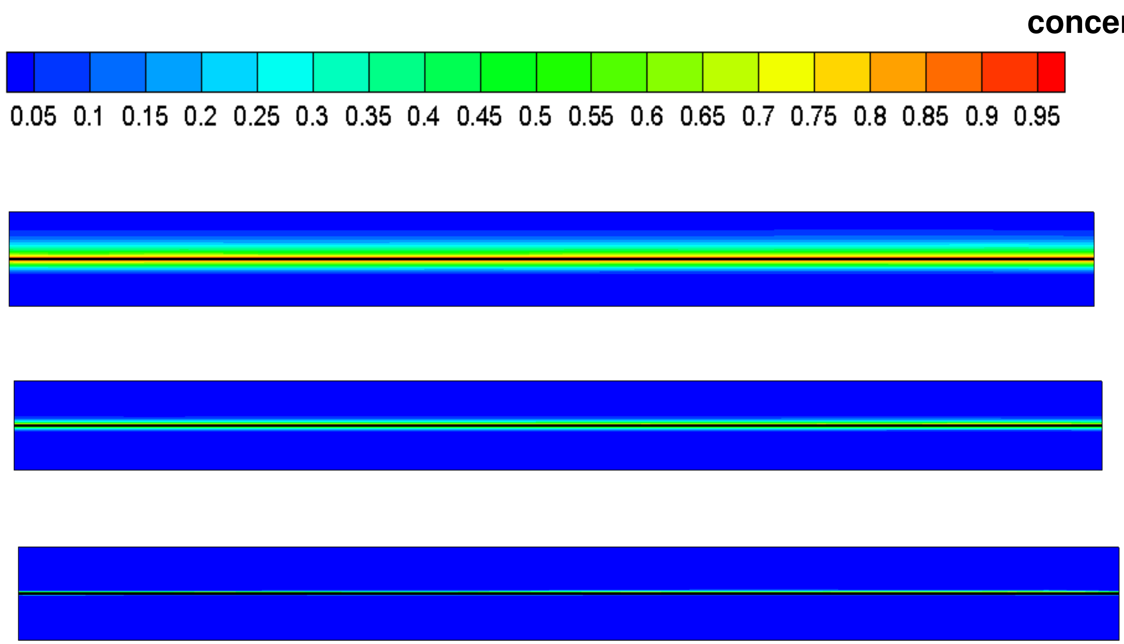
$$\delta = 5\nu_L / u_L^* \approx 2.8\ 10^{-3}\ m \qquad \delta_m = \delta\, Sc^{-1/3}$$



127 cells in the vert. direction

255 cells in the vert. direction

Mean species concentration at t=4 s, for Sc=10 (top), 100 (middle), 1000 (bottom).

Species diffusion on both sides of the interface

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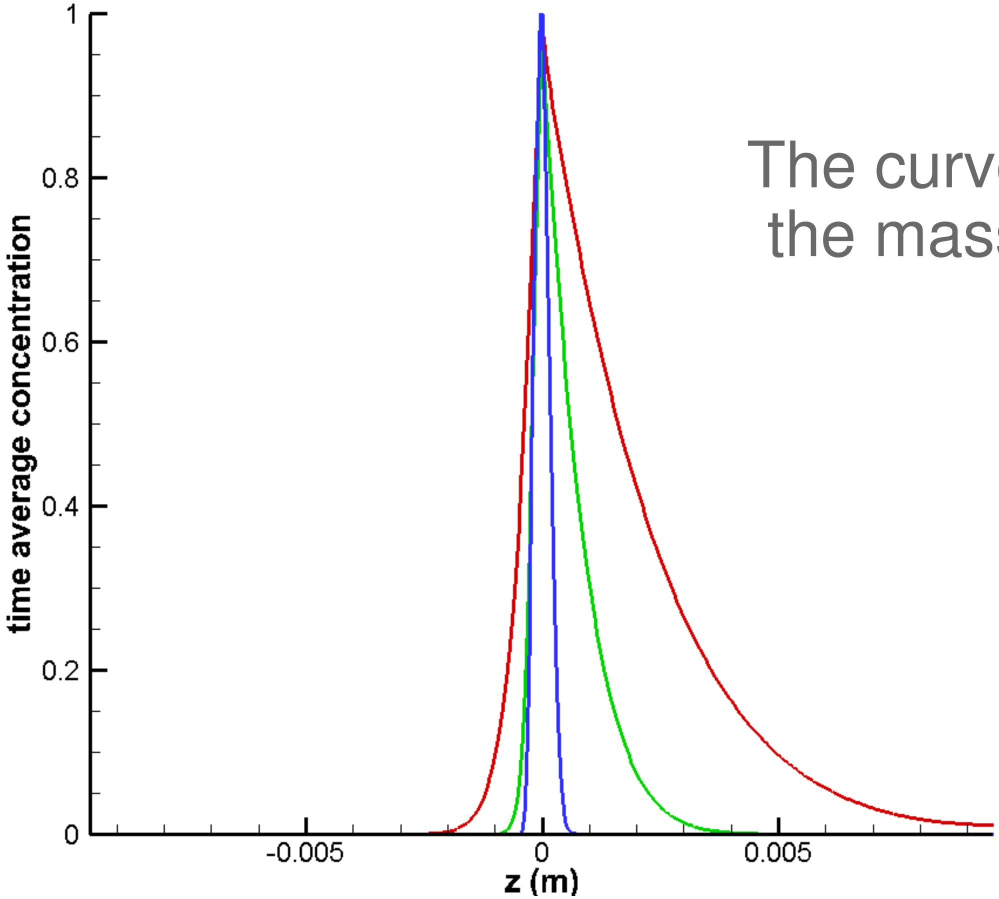

Vertical concentration profile at t=4 s, for Sc=10 (red), Sc=100 (green), Sc=1000 (blue).

The curves can be used to get the mass transfer coefficient:

$$\beta = \frac{D\left(\frac{\partial C}{\partial z}\right)_i}{(C_i - C_\infty)}$$

Shear stress, friction velocity and mass transfer coefficients

	$\tau_{i,ls}$ (Pa)	$\tau_{i,sl}$ (Pa)	u^*_{ls} (m/s)	u^*_{sl} (m/s)
t=1.4s	0.46	0.48	0.0081	0.014
t=4s	0.23	0.26	0.0057	0.01
t=6s	0.22	0.22	0.0055	0.0092

ls: liquid steel.

sl: slag.

	Mass transfer coefficient, steel side ($m.s^{-1}$)	Mass transfer coefficient, slag side, ($m.s^{-1}$)
Sc=10	4.94E-05	4.23E-04
Sc=100	1.16E-05	1.33E-04
Sc=1000	1.37E-06	2.81E-05

Mass transfer coefficients, t = 4 s.

Mass transfer coefficient depending on Sc

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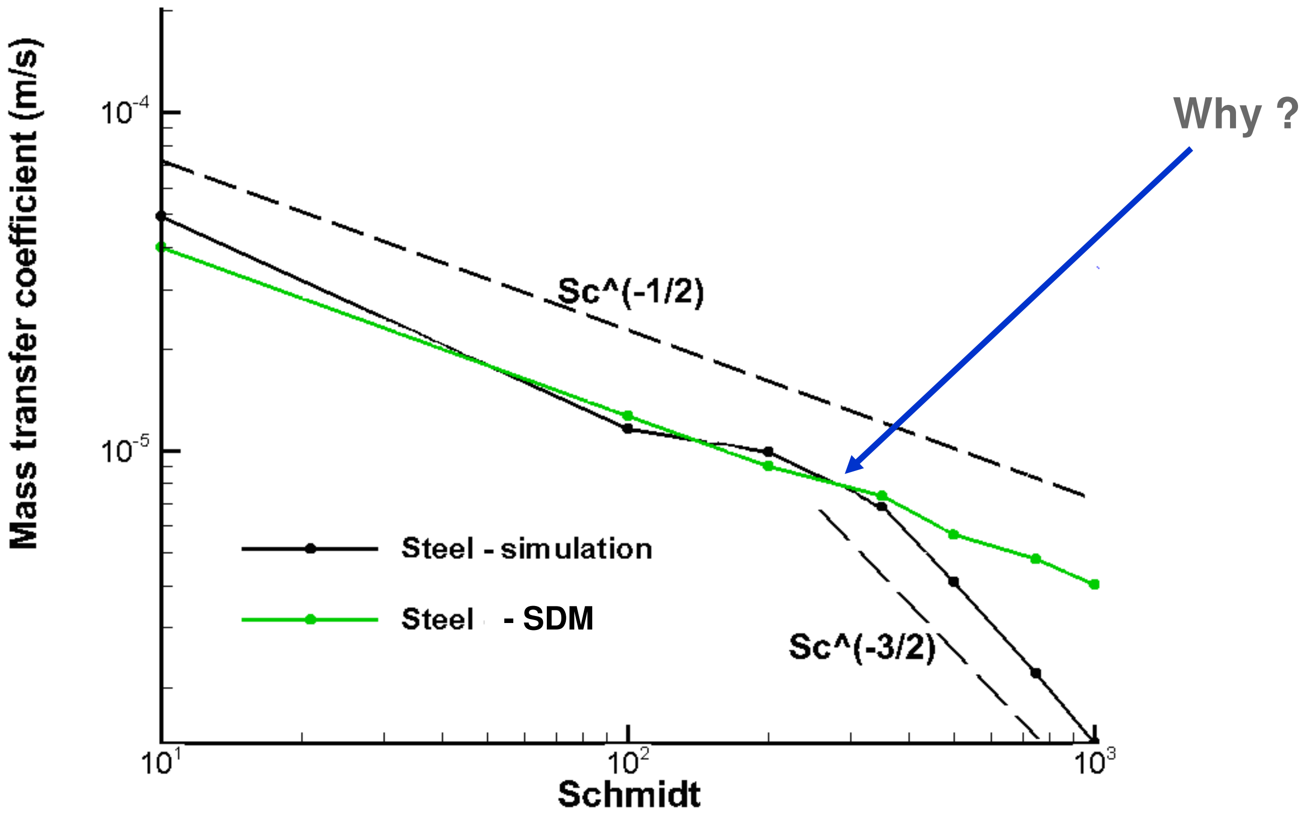

Dependence of mass transfer on Schmidt number, liquid steel side.

Inclusion entrapment by mushy zone

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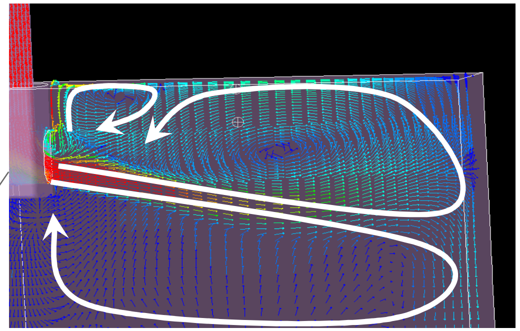
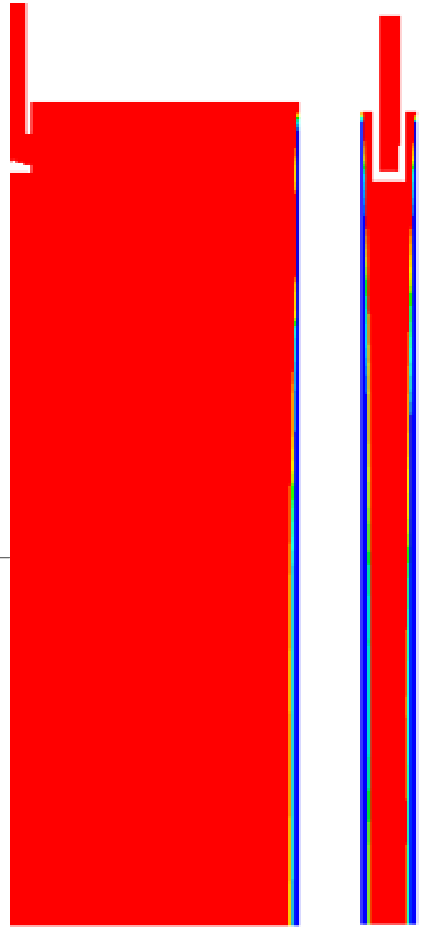
Objective: determine the number and location of inclusions entrapped by the mushy zone

- Methodology : 3-steps calculations





Fluid flow simulation

Simulation of steel solidification

Simulation of entrapment

Use of custom functions for the entrapment criterion

Cartography of the particles and their entrapment locations

Multiscale modelling & entrapment model at mushy zone

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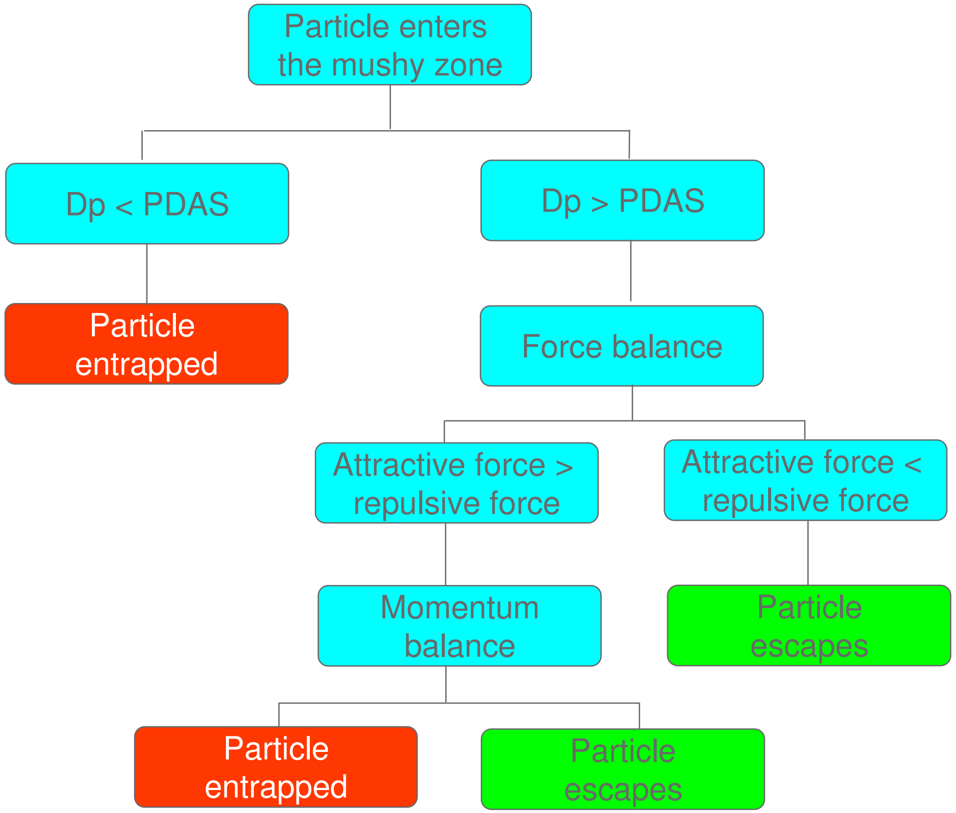
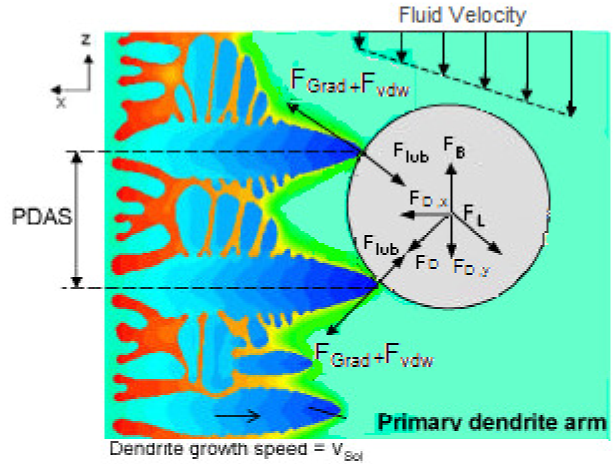


- Particles are subject to many forces:
  - Lubrication force
  - Surface gradient energy force
  - Van der Waals force
  - Buoyancy
  - Lift force
  - Drag force



Quan Yuan, *Transient Study of Turbulent Flow and Particle Transport During Continuous Casting of Steel Slabs,* Ph.D. thesis, University of Illinois at Urbana-Champaign, IL, 2004.

Lagrangian tracking of inclusions

PDAS evolution

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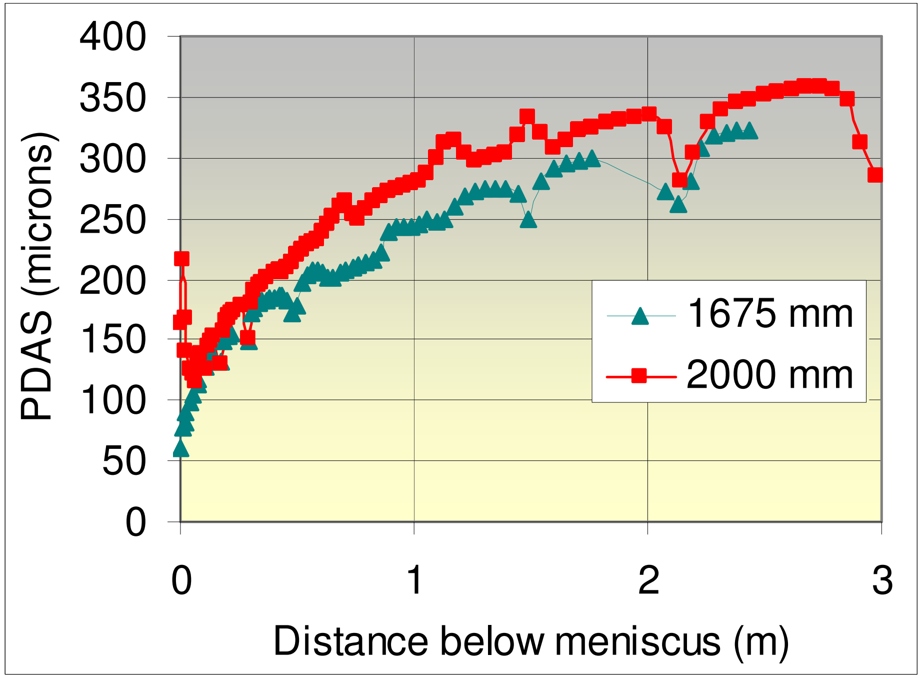
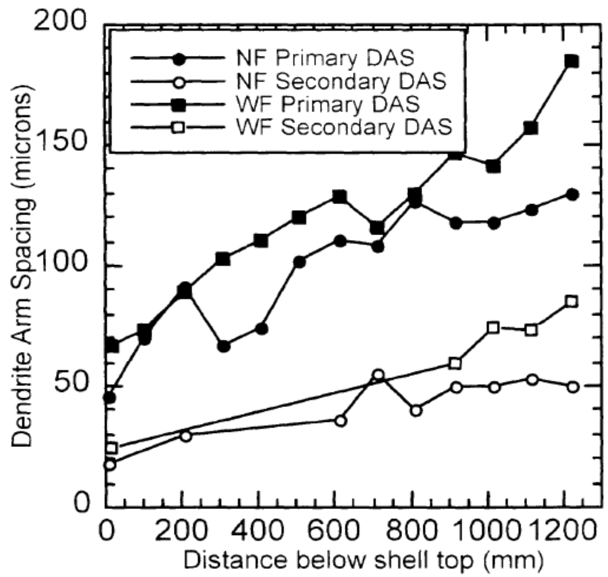
PDAS predicted:



Measured PDAS:



$$PDAS = \sqrt{\frac{3(T_{liq} - T_{sol})}{G}} \cdot \sqrt{r_d}$$

r_d: dendrite tip radius

G is the thermal gradient in the mushy zone

Exemple 2: inclusions entrapment in the mold

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Repartition of inclusions entrapment:

		W = 1675 mm	W = 2000 mm
d_p = 50 - 100 µm	Entrapped by slag	8%	8%
	Entrapped by solidification front	84%	83%
	Reaching mold lower outlet	8%	9%
d_p = 500 µm	Entrapped by slag	98%	60%
	Entrapped by solidification front	2%	40%
	Reaching mold lower outlet	0%	0%

⇨ No impact of slab width on smaller inclusions entrapment

⇨ 40% of large inclusions are entrapped by the solidification front for W=2000 mm: in good agreement with slivers industrial trends

Conclusion

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- Multiphase modelling is becoming more and more mature and is widely used for steelmaking process optimization – still some limitations for multiphysic problems
- Local refining of the mesh: attractive method to deal with multiscale problem but meshless techniques are naturally efficient
- When local mechanisms are depending on mesoscopic phenomenon: one-way coupling from the cell to the micro-scale
- More and more difficult to get data for the validation