Diffusion of mass across steel/slag interfaces

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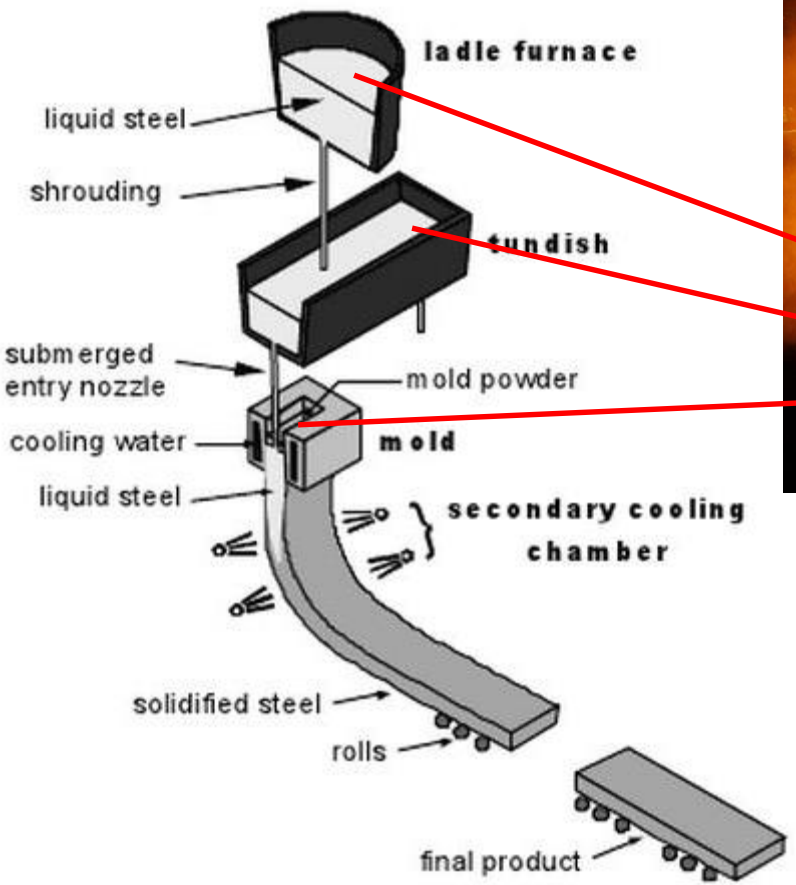
This work is granted by Arcelor-Mittal Research (Pascal Gardin)

Typical problems of interest



Mass transfer at the steel/slag interface

Interfaces – turbulent multiphase flows – surface tension – tranfer of species at the interface

How to model liquid-steel flows with slag interface and mass transfer ? Low Schmidt numbers in liquid metals

Objectives of the work

- Perform direct numerical simulation of two-phase flows with deformable interfaces and mass diffusion at interfaces

- Extend the work of mass diffusion across simple shape liquid-liquid interfaces (such as steel/slag) for topologies and configurations using realistic interface deformations

- Characterize mass transfer rate and mass transfer coefficients for realistic configurations

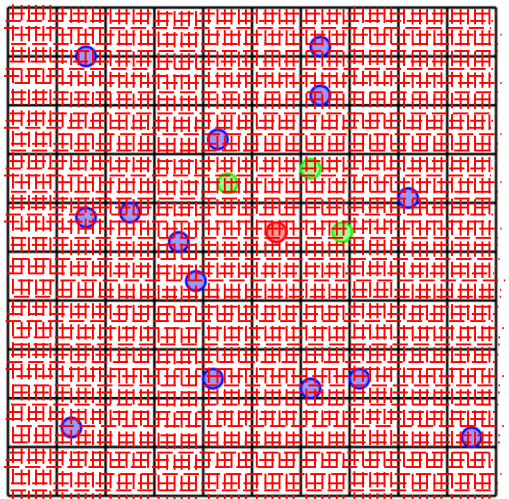
- Consider high Schmidt numbers as in casting processes

- Compare numerical mass transfer laws to existing laws of the literature, that have been validated for Sc<100

- The final goal is to use obtained numerical laws of mass transfer coefficient in macroscopic process models of Arcelor-Mittal

General numerical methods (Vincent et al. JCP 2010, 2011)

- Structured orthogonal staggered curvilinear grids, finite volumes and centered schemes
- Various Volume Of Fluid VOF methods for interface tracking
- Penalty methods for boundary conditions, obstacle and constrainsts
- DNS/LES modeling of turbulence (Smagorinsky, TKE, Mixed scale approaches)
- Direct / iterative Bi-CGSTAB II solvers + preconditionning
- Parallel implementations (up to 512 processors and 100 million points for multiphase flows) – grid decomposition into several Cartesian parts in each space direction



Modeling mass transfers at a steel/slag interface under turbulent flow regime (Caruyer et al. Surf. Coat. Tech. 2009)

$$\frac{\partial p}{\partial t} + \frac{1}{\chi_T}\nabla.u = 0$$

$$\tilde{\rho}\left(\frac{\partial u}{\partial t} + (u.\nabla)u\right) = \tilde{\rho}\mathbf{g} - \nabla\left(p + \frac{\tau}{\chi_T}\nabla\cdot u\right) + \nabla.\left(\tilde{\mu}\left(\nabla u + \nabla^T u\right)\right) + \mathbf{F}_{TS}$$

$$\frac{\partial C}{\partial t} + (u.\nabla)C = 0$$

$$\frac{\partial \psi_i}{\partial t} + (u.\nabla)\psi_i = \nabla\cdot\left[\tilde{D}_i\nabla\psi_i\right]$$

$$\tilde{\rho} = C\Omega_{\rho,w}(T) + (1-C)\left[\psi_a\Omega_{\rho,a}(T) + (1-\psi_a)\Omega_{\rho,p}(T)\right]$$

$$\tilde{\mu}_m = C\Omega_{\mu,w}(T) + (1-C)\left[\psi_a\Omega_{\mu,a}(T) + (1-\psi_a)\Omega_{\mu,p}(T)\right]$$

$$\tilde{\lambda} = C\Omega_{\lambda,w}(T) + (1-C)\left[\psi_a\Omega_{\lambda,a}(T) + (1-\psi_a)\Omega_{\lambda,p}(T)\right]$$

$$\tilde{C}_p = C\Omega_{C_p,w}(T) + (1-C)\left[\psi_a\Omega_{C_p,a}(T) + (1-\psi_a)\Omega_{C_p,p}(T)\right]$$

$$\tilde{D} = CD_w + (1-C)\left[\psi_a D_a + (1-\psi_a)D_p\right]$$

Surface tension

$$\mathbf{F}_{TS} = \sigma\kappa n_i\delta_i$$

LES modeling

$$\tilde{\mu} = \tilde{\mu}_m + \mu_t$$

$$\mu_T = \rho C_S^{2\alpha} C_{TKE}^{1-\alpha}\overline{\Delta}^{1+\alpha}\left(2S_{ij}S_{ij}\right)^{\alpha/2}\left(\frac{1}{2}\overline{\mathbf{u}'\mathbf{u}'}\right)^{\frac{1-\alpha}{2}}$$

$$\tilde{D}_i = \tilde{D}_{i,m} + \frac{\mu_t}{\rho Sc_t}$$

Not depending on temperature nor in species concentration

In our case, just on the VOF fraction C

Specific numerical methods

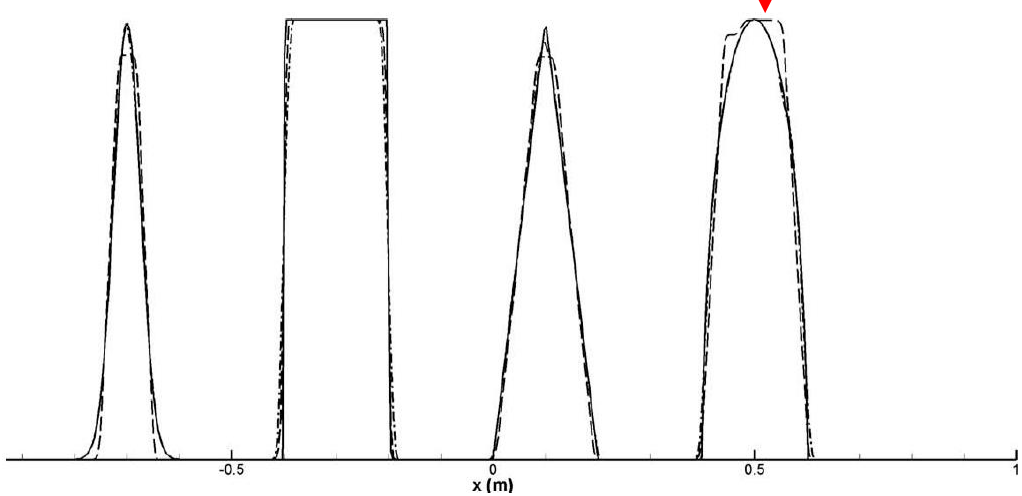
Surface tension: CSF Brackbill model + Smooth VOF (Brackbill et al. JCP 1992, Pianet et al. IJMF 2010)

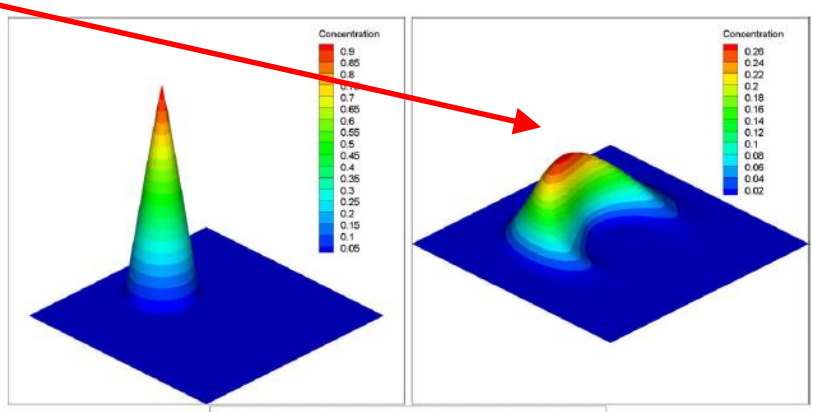
$$\mathbf{F}_{ST} = \sigma\kappa\mathbf{n}_i\delta_i = \sigma\nabla\cdot\left(\frac{\nabla C^S}{\|\nabla C^S\|}\right)\nabla C^S$$

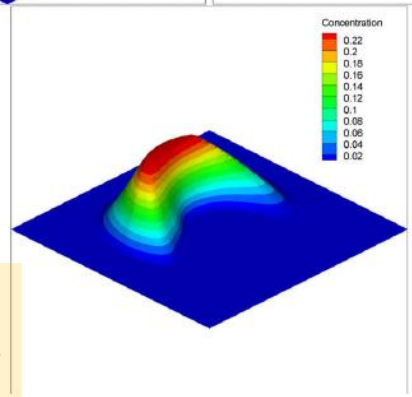
$$-\nabla\cdot\tau_d^*\nabla C^{S,k+1} + C^{S,k+1} = F^k$$

$$F^{k+1} = C^{S,k+1}$$

Transport equation for species: Lax-Wendroff TVD scheme (Vincent et al. IJNMF 1999, Vincent et al. JCP 2010)



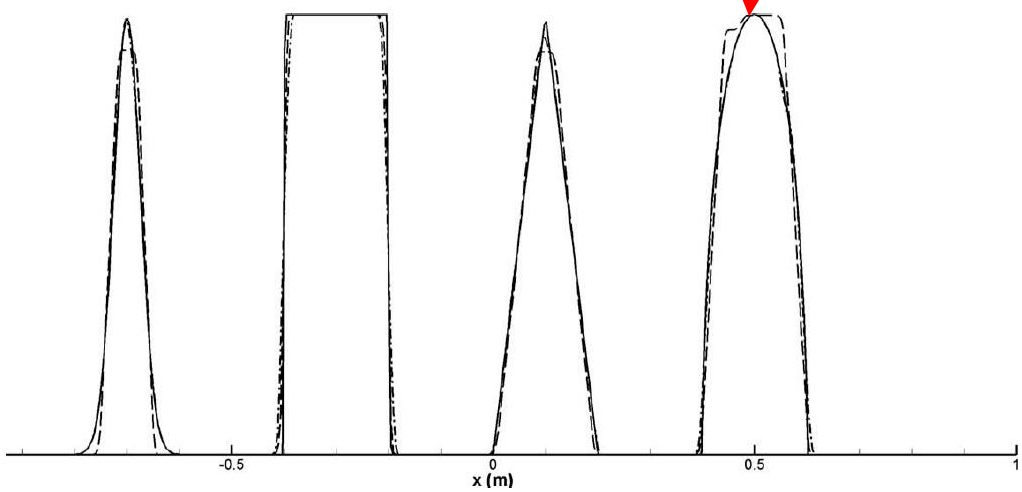


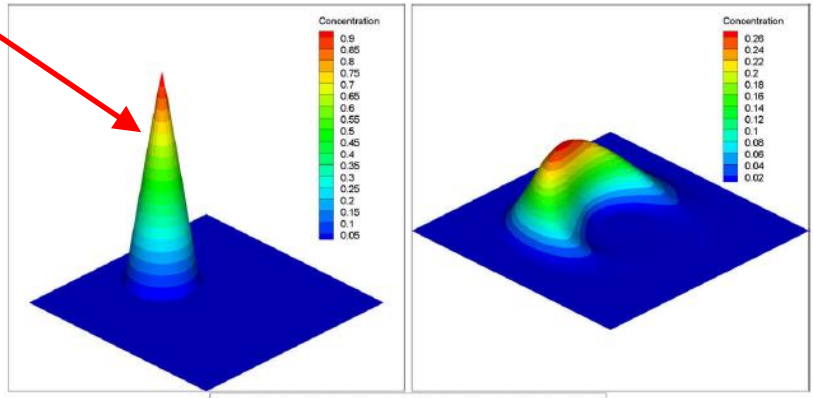


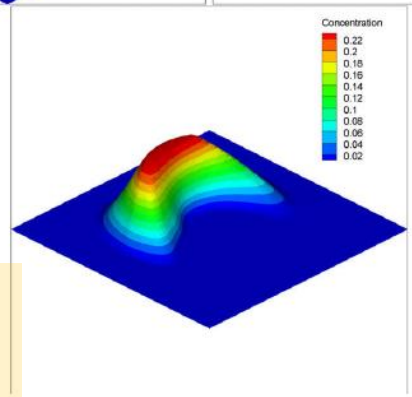
The best scheme in the literature but too compressive near steep gradients or too diffusive when shearing is driving the flow

Specific numerical methods

Transport equation for species: new VOF-SM scheme (Vincent et al. JCP 2010)







Better than the Lax-Wendroff TVD scheme or any Eulerian scheme devoted to hyperbolic equations

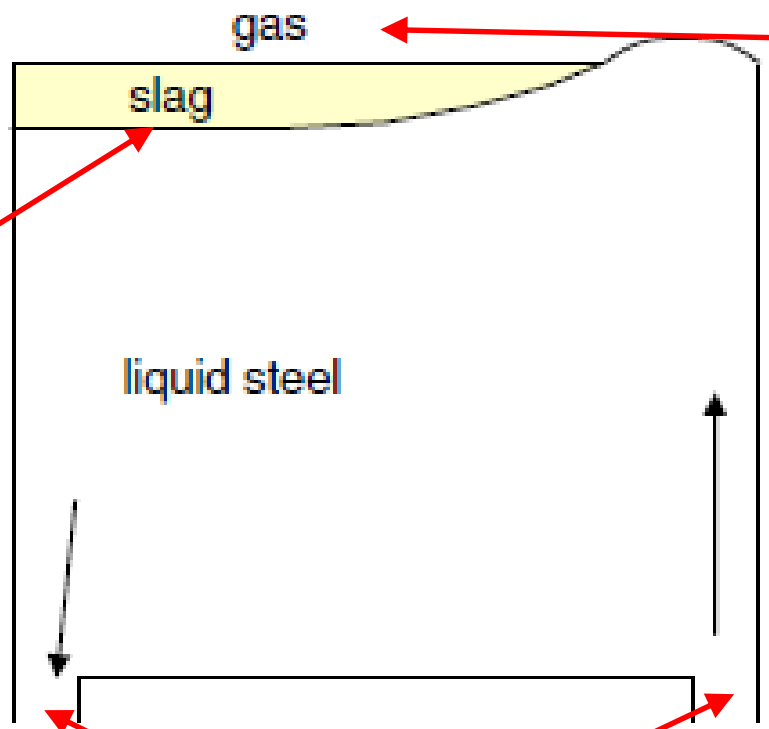
VOF-SM is a Lagrangian technique for solving an Eulerian transport equation

No more diffusive, no more compressive, no more dispersive
More expensive in CPU time than Eulerian schemes

Simulation of a 2D steel/slag interface problem

Gas has little influence on steel/slag dynamics as no air droplet are incorporated into liquids

Mass transfer at interface steel/slag interface



Gas medium is discarded in our simulations

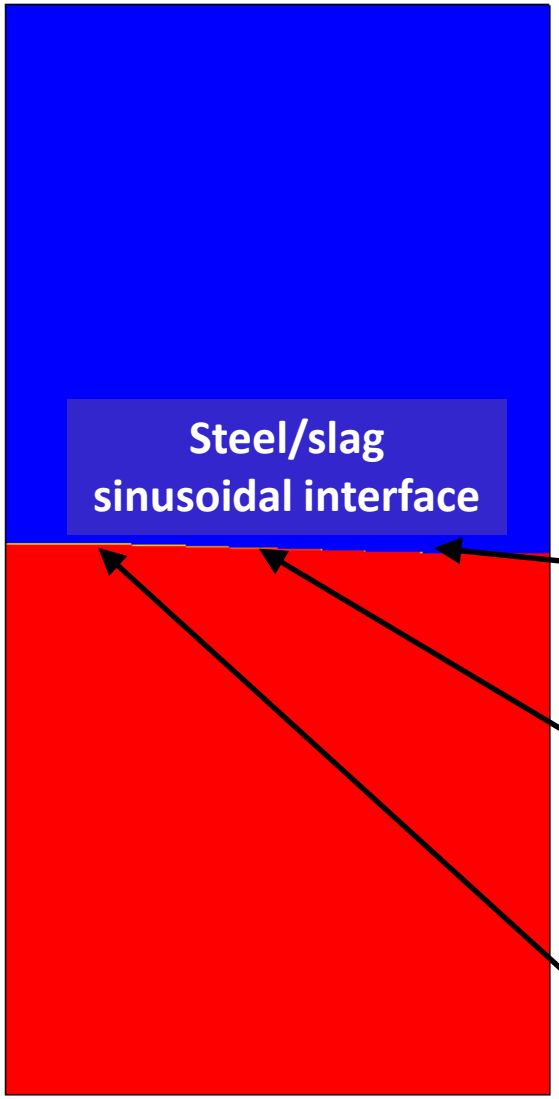
Injection of liquid on one part and extraction on the other part

Injection Re=40000 Injection We=158

Initially, steel/slag interface is flat

A kind of sloshing wave is generated from right to left under steel injection/extraction

Validation of hydrodynamics

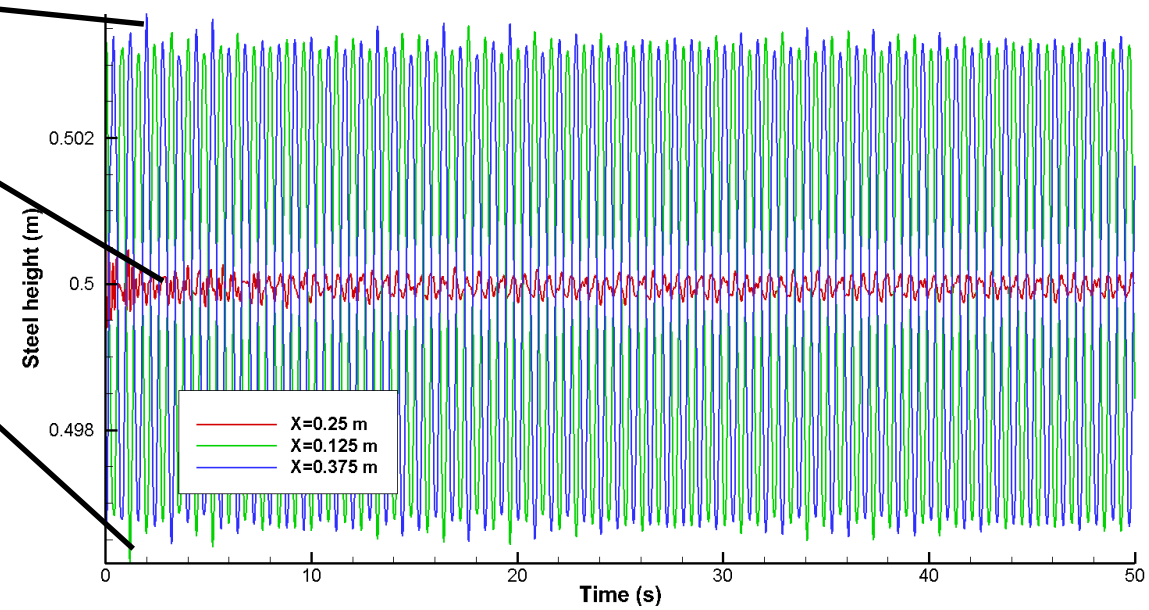


100 x 800 grid

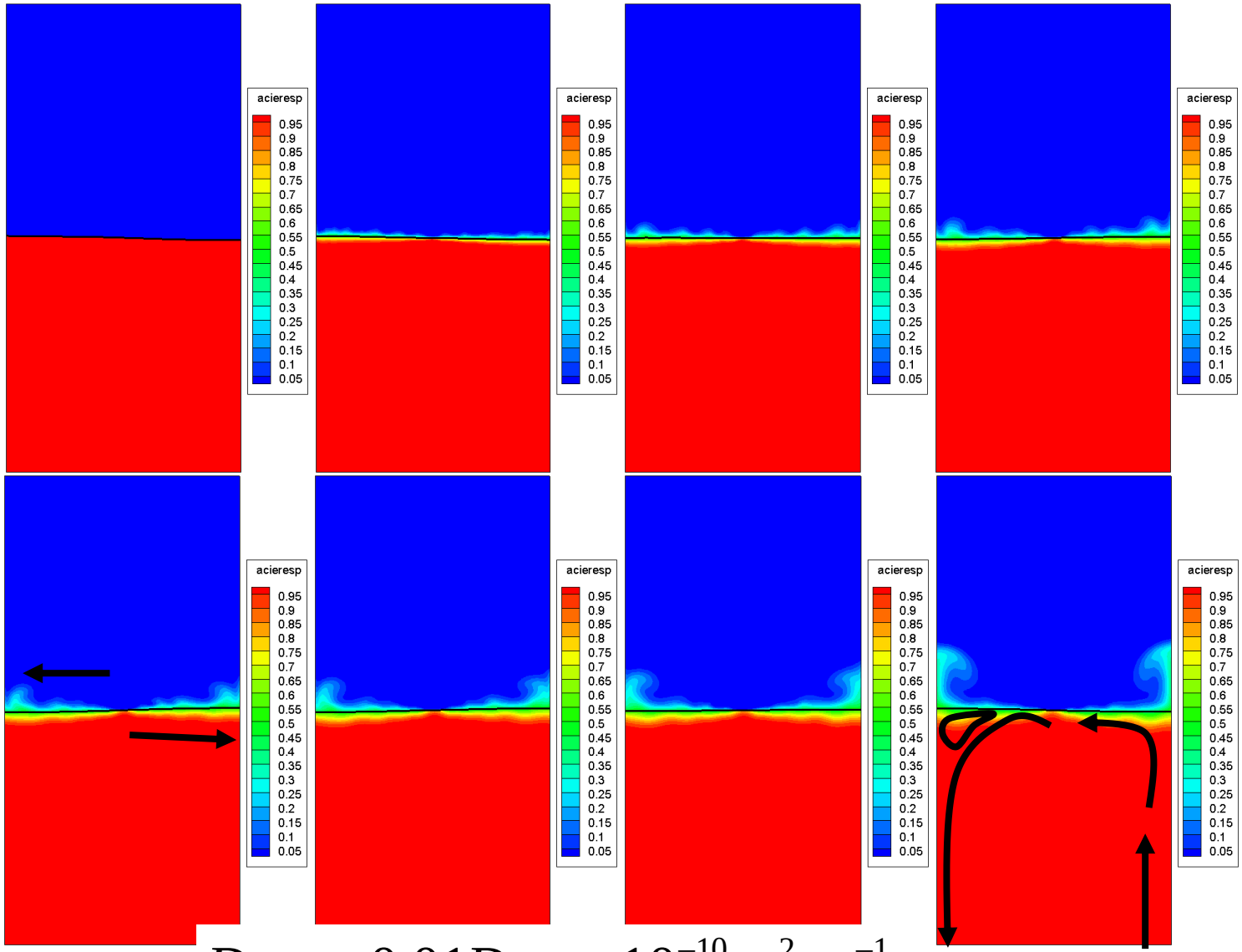
Simulation over 50s

Analytical frequency f is 0.8 s and a value of 0.806s is found numerically

$$f = \frac{1}{2\pi}\sqrt{\pi g \frac{i}{L} th(\pi H \frac{i}{L})}$$



Hydrodynamics and mass diffusion of the 2D test problem



Sc=1000

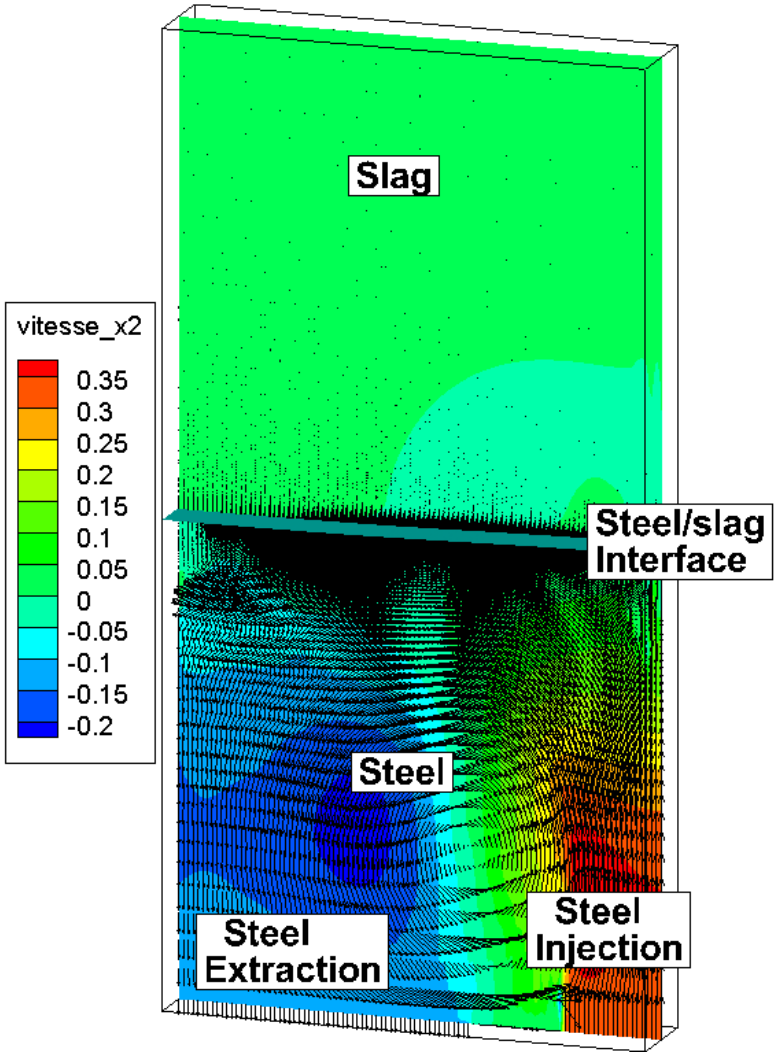
100 x 800 grid

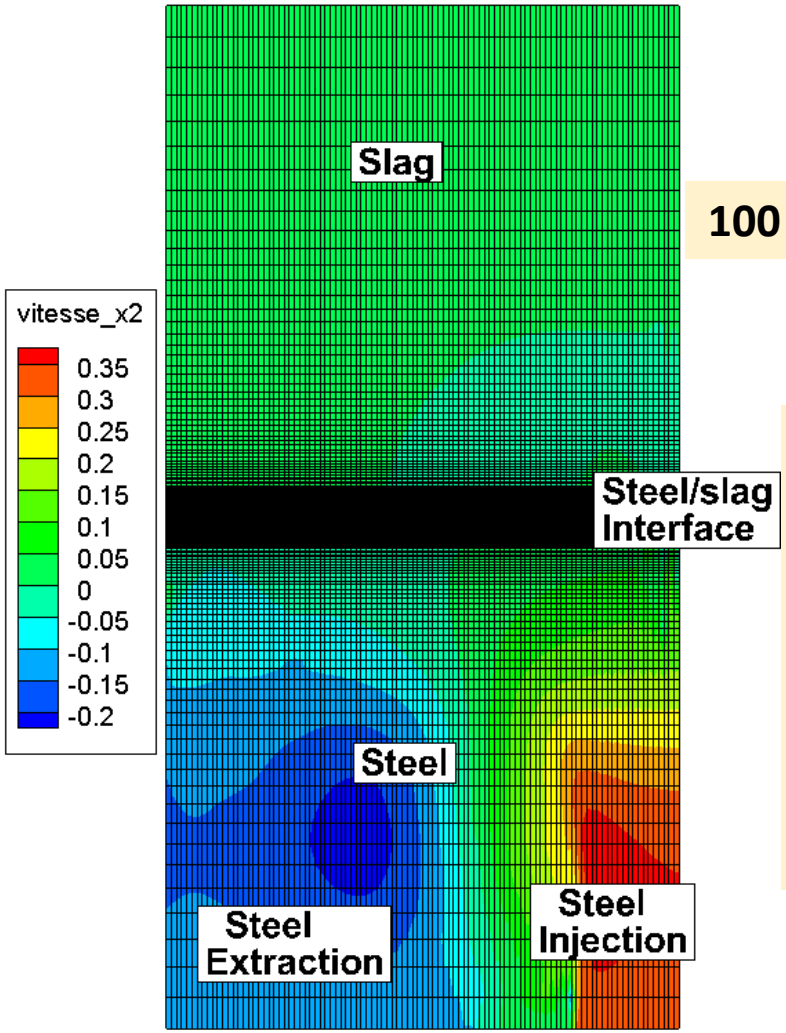
Kind of sloshing behaviour at interface with mass transfer over time

Diffusion is faster in slag than in steel

$$D_{steel} = 0.01 D_{slag} \approx 10^{-10}\, m^2 \cdot s^{-1}$$

Hydrodynamics and mass diffusion of the 3D test problem





Sc=1000

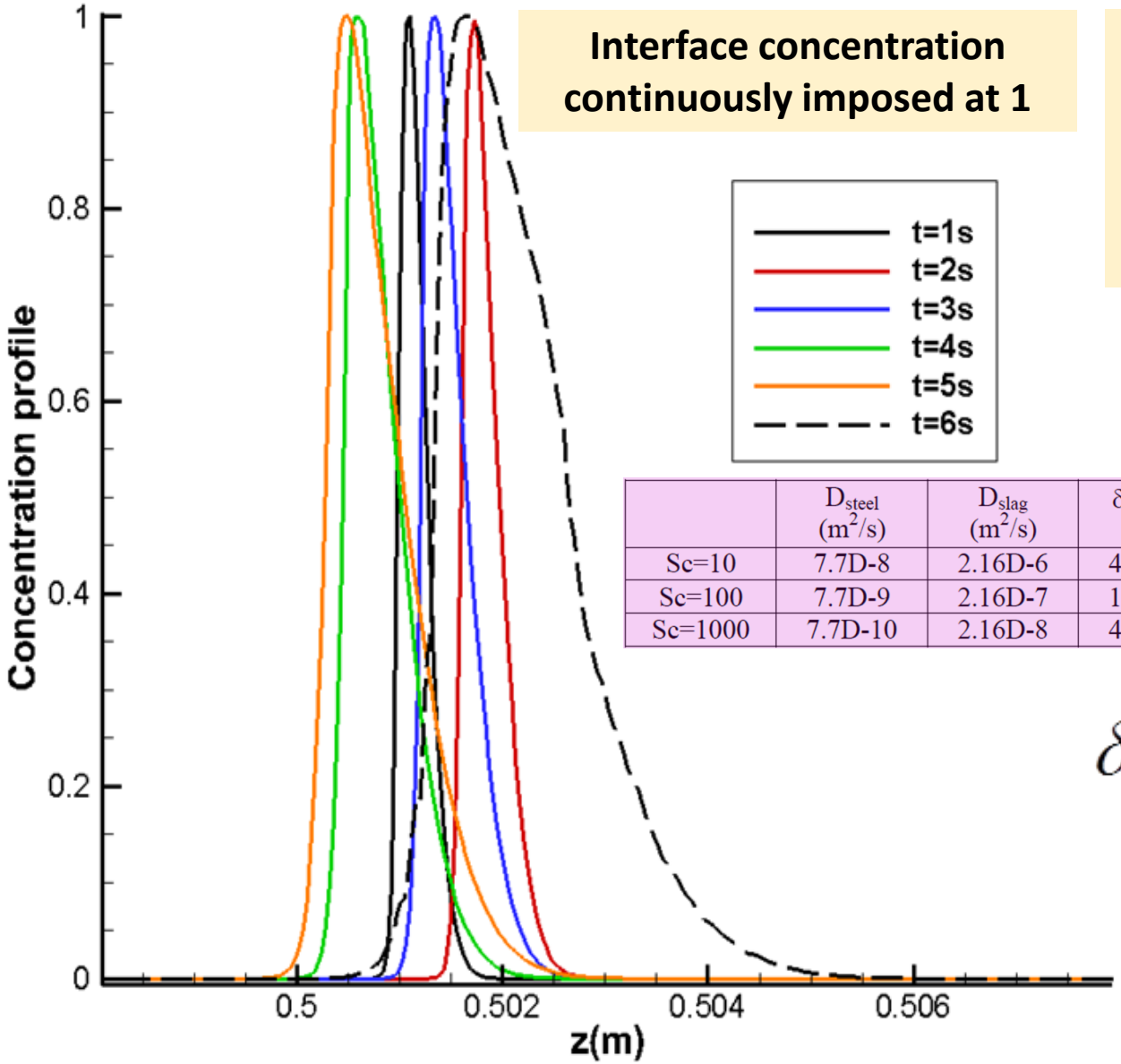
100 x 20 x 400 grid

Same kind of behaviour than in 2D

Comparison between 2D and 3D results

$$D_{steel} = 0.01 D_{slag} \approx 10^{-10}\, m^2 \cdot s^{-1}$$

Estimate of mass transfer coefficient at liquid-slag interface



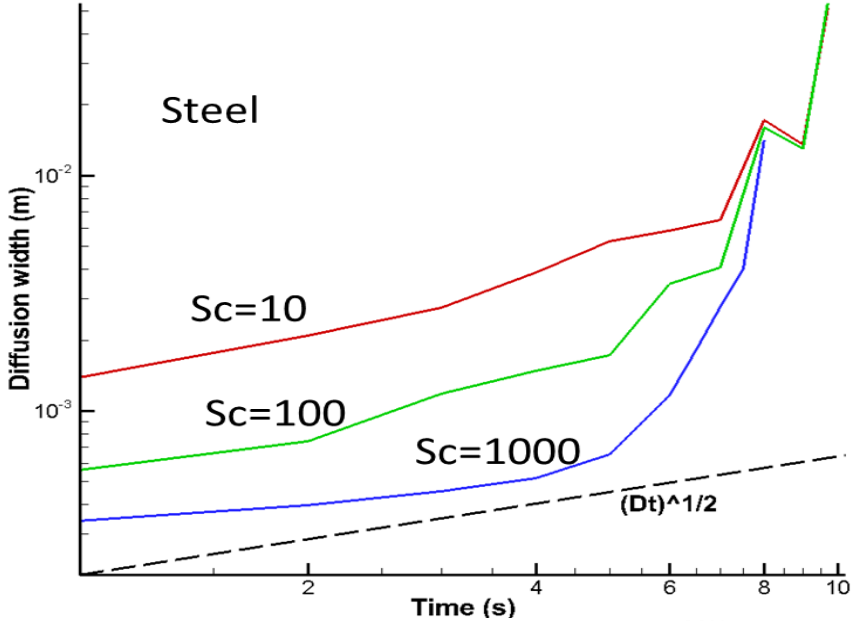
Interface concentration continuously imposed at 1

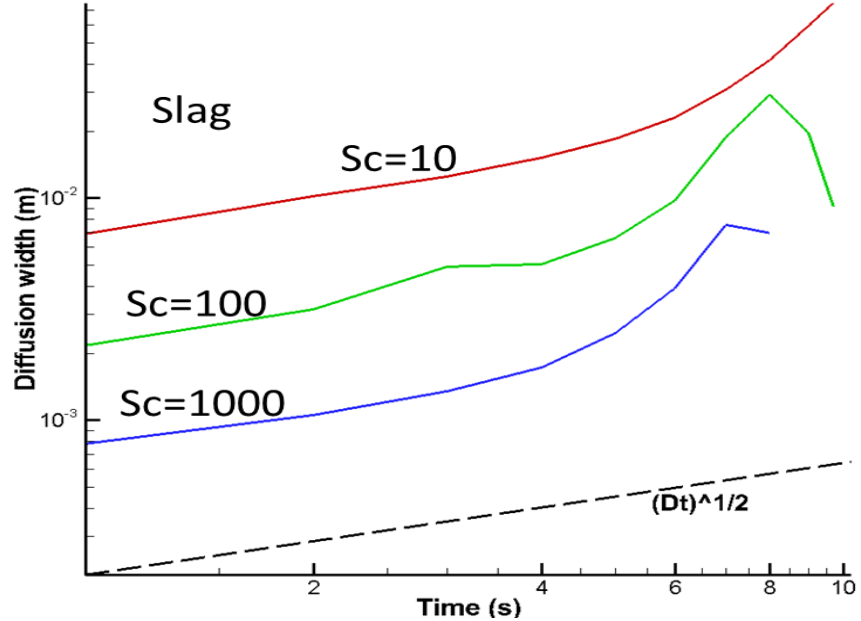
Continuity of $\mu \frac{\partial u}{\partial z}$ has ben checked

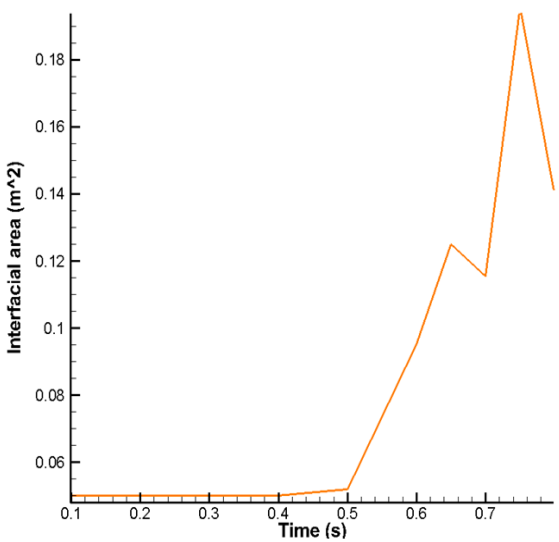
	D_{steel} (m^2/s)	D_{slag} (m^2/s)	$\delta_{num,steel}$ (m)	$\delta_{num,slag}$ (m)	$\delta_{th,steel}$ (m)	$\delta_{th,slag}$ (m)
Sc=10	7.7D-8	2.16D-6	4.00D-3	2.17D-2	4.14D-3	2.19D-2
Sc=100	7.7D-9	2.16D-7	1.30D-3	6.67D-3	1.31D-3	6.93D-3
Sc=1000	7.7D-10	2.16D-8	4.48D-4	2.14D-3	4.14D-4	2.19D-3

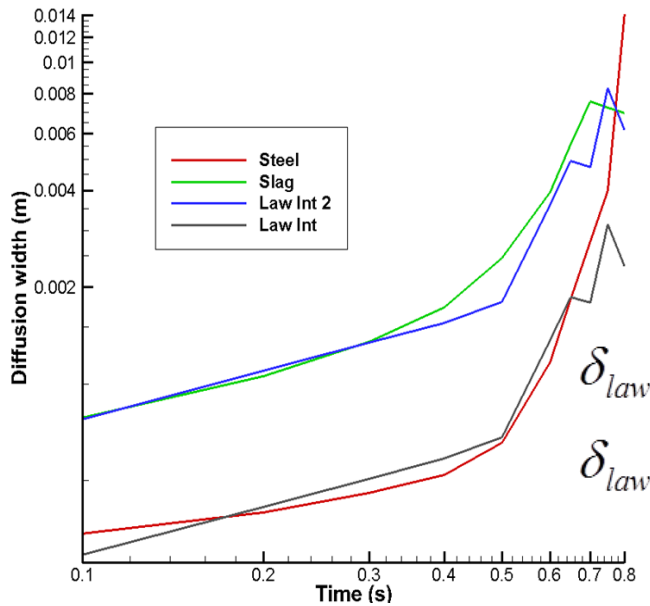
$$\delta_{th} = \sqrt{D\tau}$$

Estimate of mass transfer coefficient at liquid-slag interface







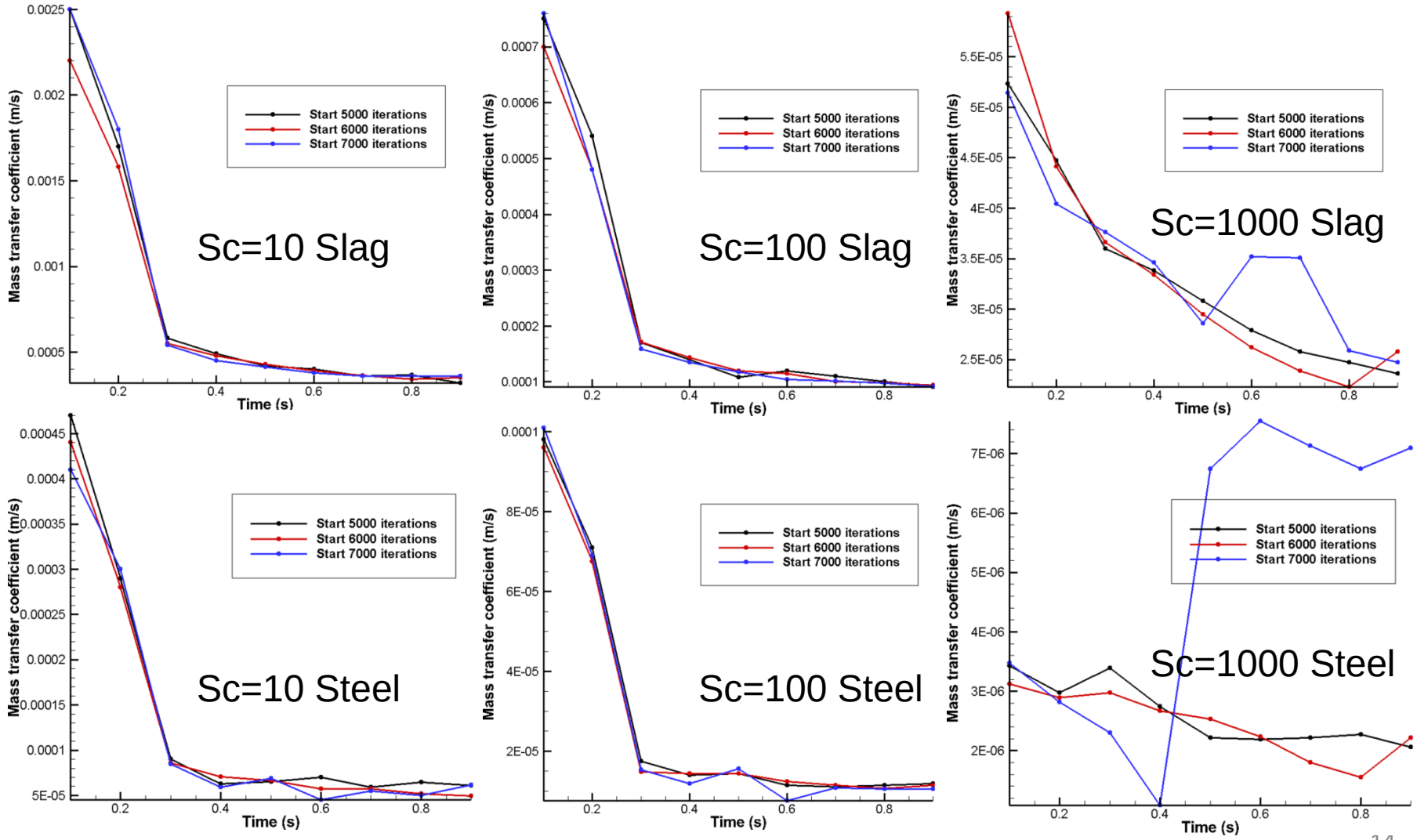


$$\delta_{lawint} = Sc^{1/2}\sqrt{D\tau}\Sigma(t)/(3\Sigma_0)$$

$$\delta_{lawint2} = Sc^{1/2}\sqrt{D\tau}\Sigma(t)/(6\Sigma_0)$$

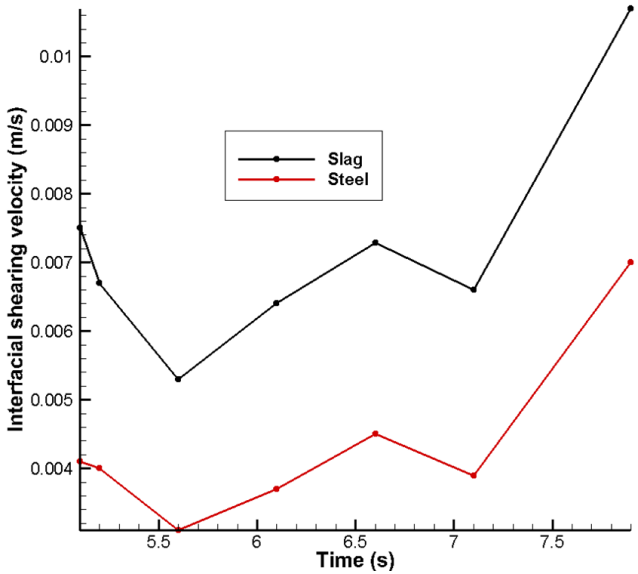
Estimate of mass transfer coefficient at liquid-slag interface

Interface concentration reinitialized every 1 s and imposed at 1



Estimate of mass transfer coefficient at liquid-slag interface

Interface concentration reinitialized every 1 s and imposed at 1



Mass transf. Coeff.	Sc=10	Sc=100	Sc=1000
Slag res num	3^{e-4}	1^{e-4}	2.5^{e-5}
Steel res num	5^{e-5}	1.5^{e-5}	4^{e-6}
Slag loi diff	1.5^{e-3}	5^{e-4}	1.55^{e-4}
Steel loi diff	3^{e-4}	9.2^{e-4}	2.92^{e-5}
Slag Banerjee 0.108	2.4^{e-4}	7.6^{e-5}	2.4^{e-5}
Steel Banerjee 0.108	1.4^{e-4}	4.3^{e-5}	1.4^{e-5}
Steel Banerjee 0,038	4.8^{e-5}	1.52^{e-5}	4.8^{e-6}
Slag Fortescue	1.9^{e-4}	6.1^{e-5}	1.9^{e-5}
Steel Fortescue	2.66^{e-5}	8.4^{e-6}	2.66^{e-6}
Slag Banerjee2	1.6^{e-4}	5.0^{e-5}	1.6^{e-5}
Steel Banerjee2	4.43^{e-5}	1.4^{e-5}	4.43^{e-6}

$$k_{Banerjee} = C\,Sc^{-1/2} u^*_{fric}$$

$$k_{Fortescue} = 1.07 Sc^{-1/2} u^*_{fric}\,\mathrm{Re}_T^{1/2}$$

$$k_{Banerjee2} = 0.25 Sc^{-1/2} u^*_{fric}\,\mathrm{Re}_T^{1/4}$$

$$\varphi_{c,a} = D_a \left\| \frac{1-0}{H_{G,a}} \right\| = k_a \qquad \varphi_{c,l} = D_l \left\| \frac{1-0}{H_{G,l}} \right\| = k_l$$

The interface shearing Banerjee law for mass transfer coefficient is working also for high Schmidt numbers

New result never discussed in literature

Conclusions and perspectives

- A two-phase VOF model for mass transfer at a liquid-slag interface has been designed and validated

- A new VOF-SM lagrangian scheme has been developed and validated with succes for 10<Sc<1000 in steel and slag

  it allows for simulating very small diffusion coefficients in liquid at short times without numerical diffusion

  it is the best scheme compared to existing Eulerian techniques for hyperbolic transport equations

- Various 2D and 3D steel injection problems surrounded by slag have been investigated. Sloshing motions has been highlighted and compared with success to linear theory

- Different mass transfer diffusion laws have been considered (surface divergence, shearing velocity, scalar diffusion) to scale up the small scale simulation results

  with continuous mass transfer, diffusion is controled by $KSc^{1/2}\sqrt{D\tau}$ diffusion law

  with discontinuous mass transfer over time, the mass transfer is dominated by Sc and shearing velocity at interface according to a Banerjee law

Thank you for your attention