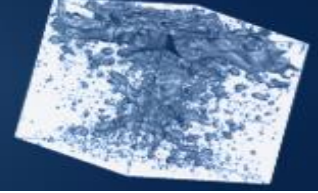




# TI 2018

5<sup>th</sup> International Conference on Turbulence and Interactions

25-29 June 2018 - Martinique



# Assessment of fluid flow and turbulence near a stratified liquid-liquid interface Implications on mass transfer coefficients

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<sup>1</sup> I2M Institute, UMR 5295, Bordeaux University, France

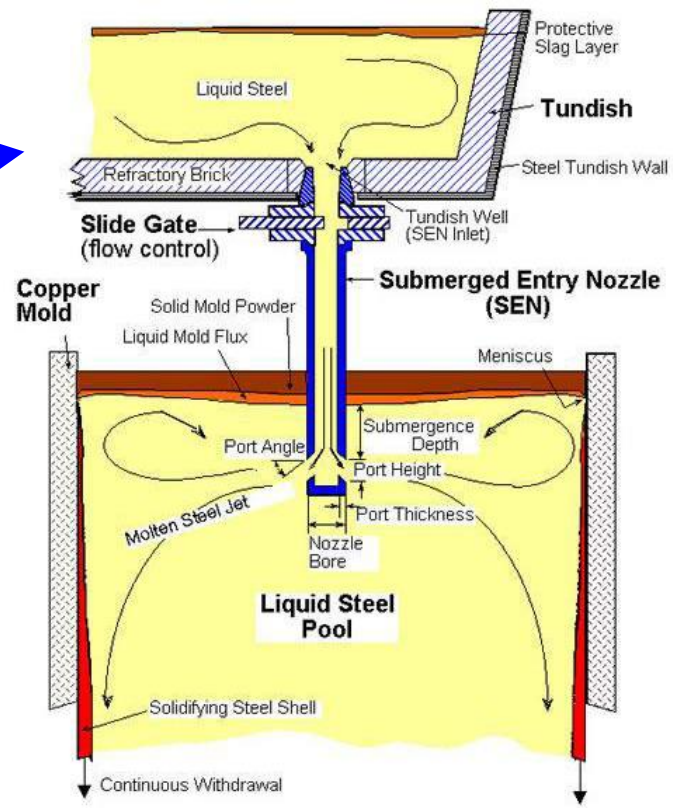
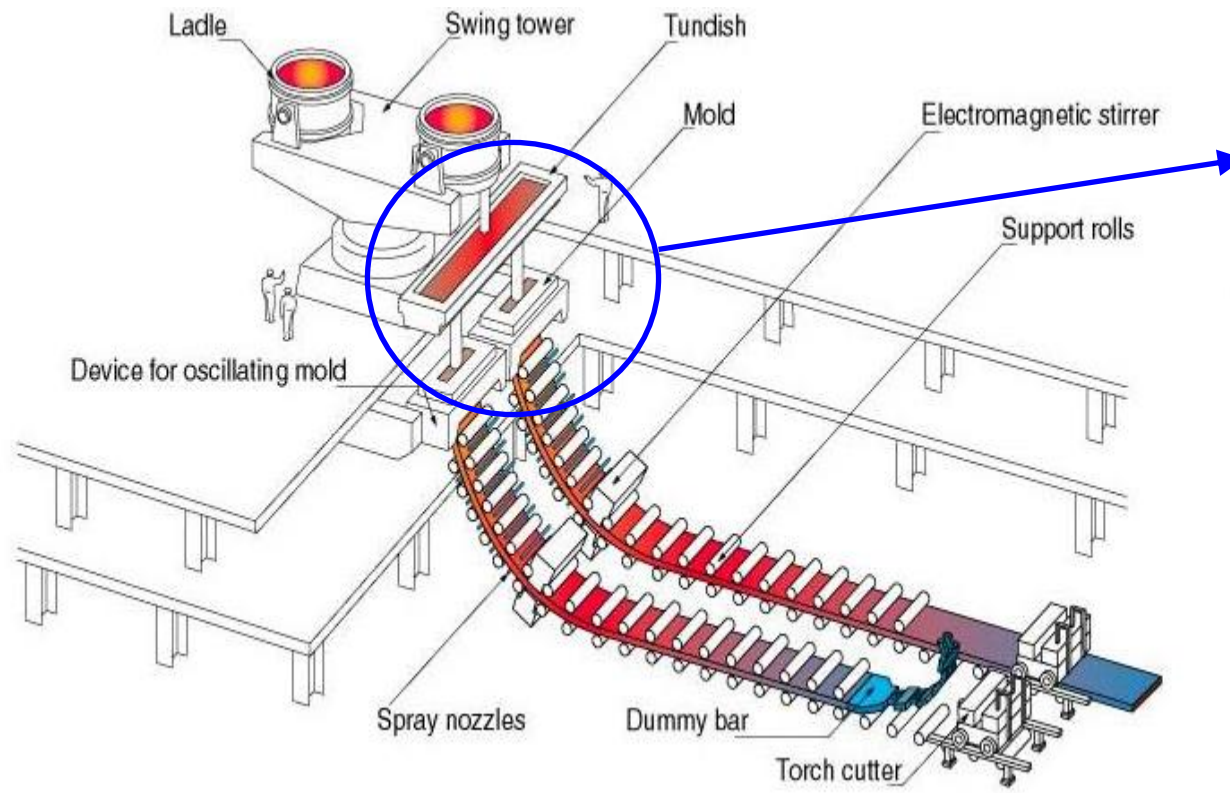
<sup>2</sup> MSME lab, UMR CNRS 8208, Paris-Est Marne-La-Vallée University, France

<sup>3</sup> Arcelor-Mittal Research, Mézières-Les-Metz, France



## Siderurgical applications

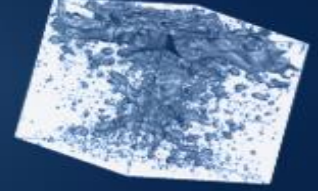
- The continuous casting machine [Campos, PhD thesis, Univ. Bordeaux, 2017]



Multiphase flow (steel, slag, argon)

Turbulent ( $Re=5000$  based on SEN diameter)

Diffusion of chemical species across steel/slag interfaces



# Modeling turbulent multiphase flows

- Incompressible volume of fluid (VOF) methods for resolved scale interfaces [Vincent *et al.*, Comput. Fluids. 2016]

$$\nabla \cdot \mathbf{u} = 0$$

$$\rho \left[ \frac{\partial \mathbf{u}}{\partial t} + \nabla \cdot (\mathbf{u} \otimes \mathbf{u}) \right] + \nabla \cdot (p \mathbf{Id} - 2\mu \mathbf{S}_D) - \rho \mathbf{g} - \gamma \kappa \mathbf{n}_i \delta_i = 0$$

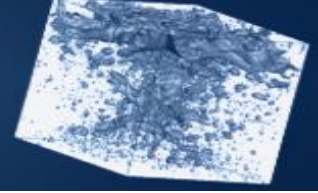
$$\frac{\partial \chi}{\partial t} + \mathbf{u} \cdot \nabla \chi = 0$$

+

**LES modeling of turbulence** with subgrid viscosity (Mixed Scale model) [Sagaut, Springer, Verlag, 1998]

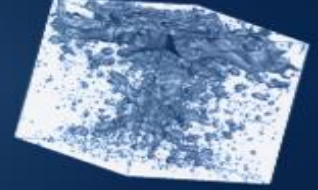
The specific two-phase subgrid LES terms are **not modelled**  
[Labourasse *et al.* Int. J. Multiphase Flow 2007] [Vincent *et al.* Comput. Fluids 2008]

No phase change is considered



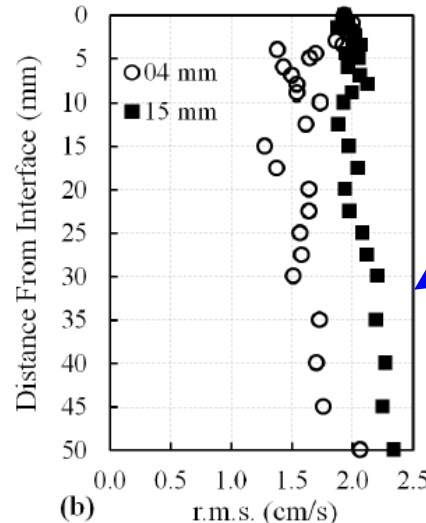
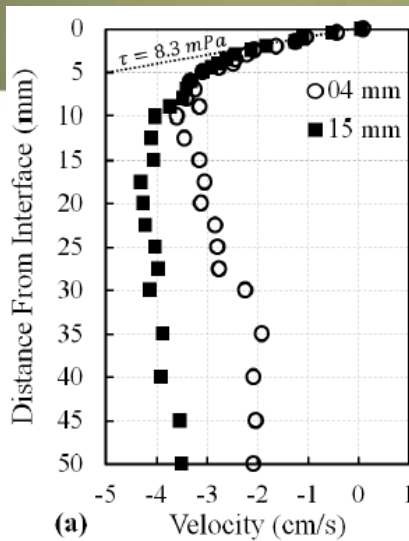
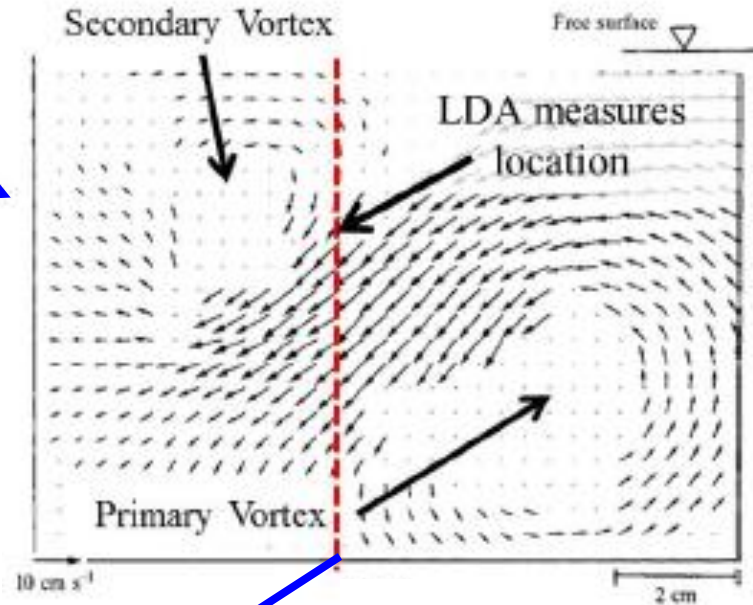
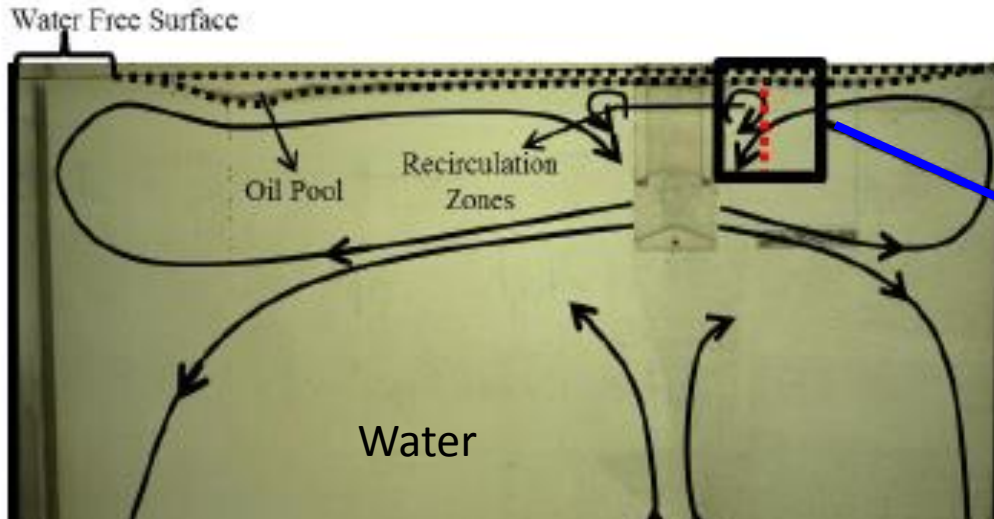
## Numerical methods

- Implicit **finite volumes**
- All velocity variables are solved in a same linear system
- Fixed Cartesian staggered meshes
- **Adams-Bashforth** time linearization of non-linear inertial terms
- Second order centered schemes in time and space
- **Adaptive augmented Lagrangian** approach for pressure-velocity coupling [Vincent *et al.* J. Comput.Phys. 2011]
- PLIC VOF [Youngs, Numer. Meth. Fluid Dyn., 1982]
- Smooth VOF for capillary effects and wetting [Guillaument, Mech. Res. Com., 2015]
- **Penalty methods** for obstacles (SEN)
- BiCGSTAB II solver [H. Van Der Vorst, SIAM J. Scientific Stat. Comput., 1992]
- MILU(0) preconditioning [I. Gustafsson, PhD Dissertation, Chalmers Univ., 1978]
- MPI // computing



## Water-oil CC experimental model

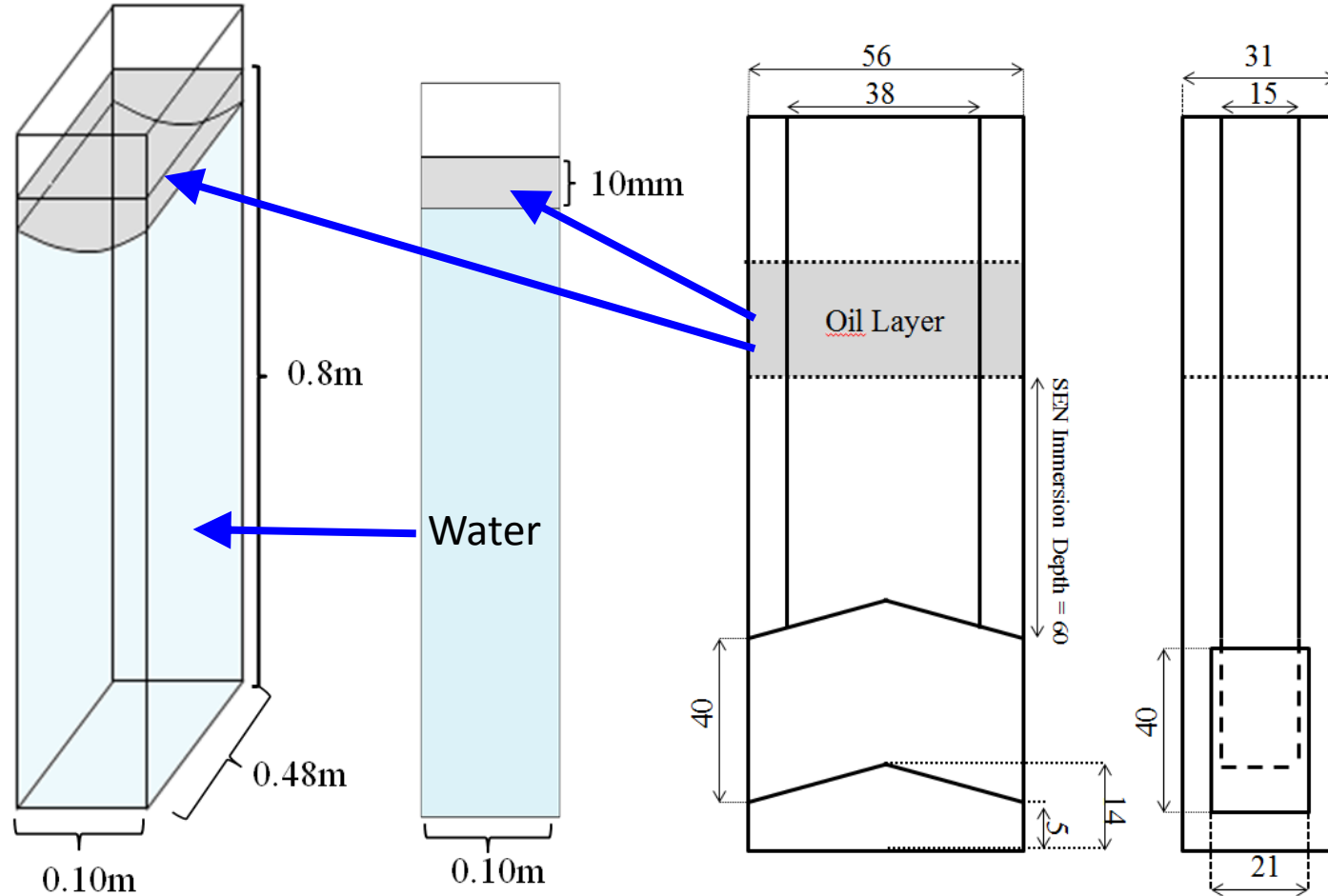
- Laser Doppler Anemometry (LDA) for velocity measurements

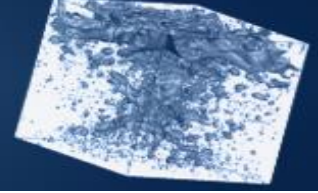


	Silicone Oil 1	Silicone Oil 2
Density (kg/m <sup>3</sup> )	970	950
Viscosity (Pa.s)	0.340	0.019
Surface Tension (×10 <sup>-3</sup> N/m) (oil/air)	21.1	20.3
Interface Tension (×10 <sup>-3</sup> N/m) (oil/water)	31.7	32.6

## Simulation of the Water-oil CC model

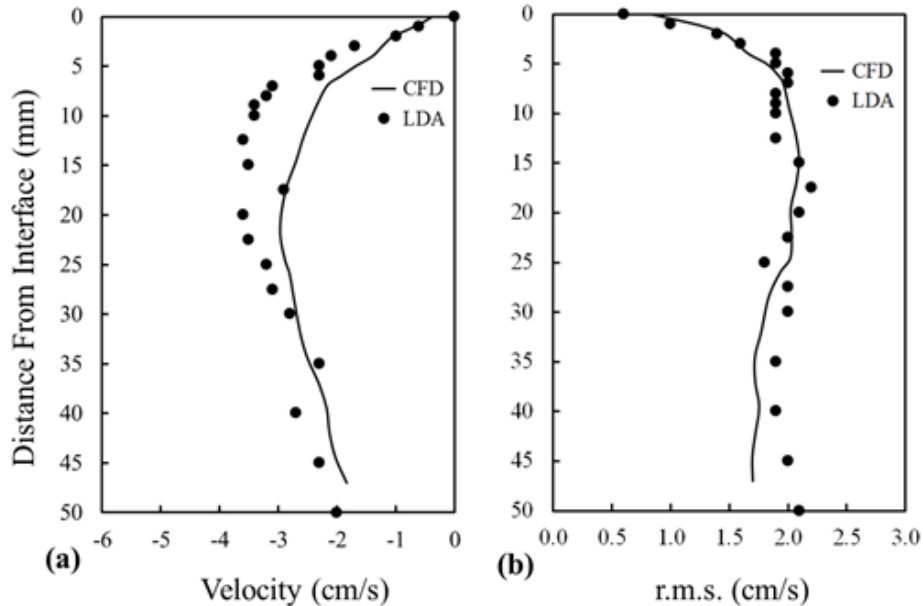
- Cartesian mesh, 1.8 million grid cells, refined at water/oil interface, 200 procs



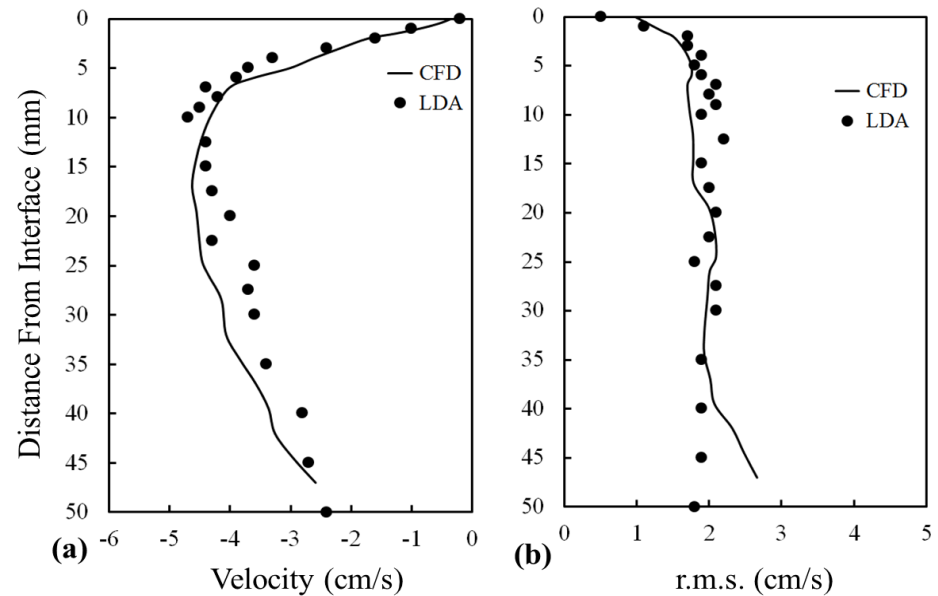


## Simulation of the Water-oil CC model

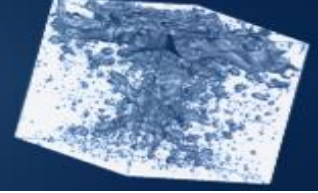
- $Q=1.6 \text{ cm}^3/\text{min}$ ,



3.5 cm from the SEN

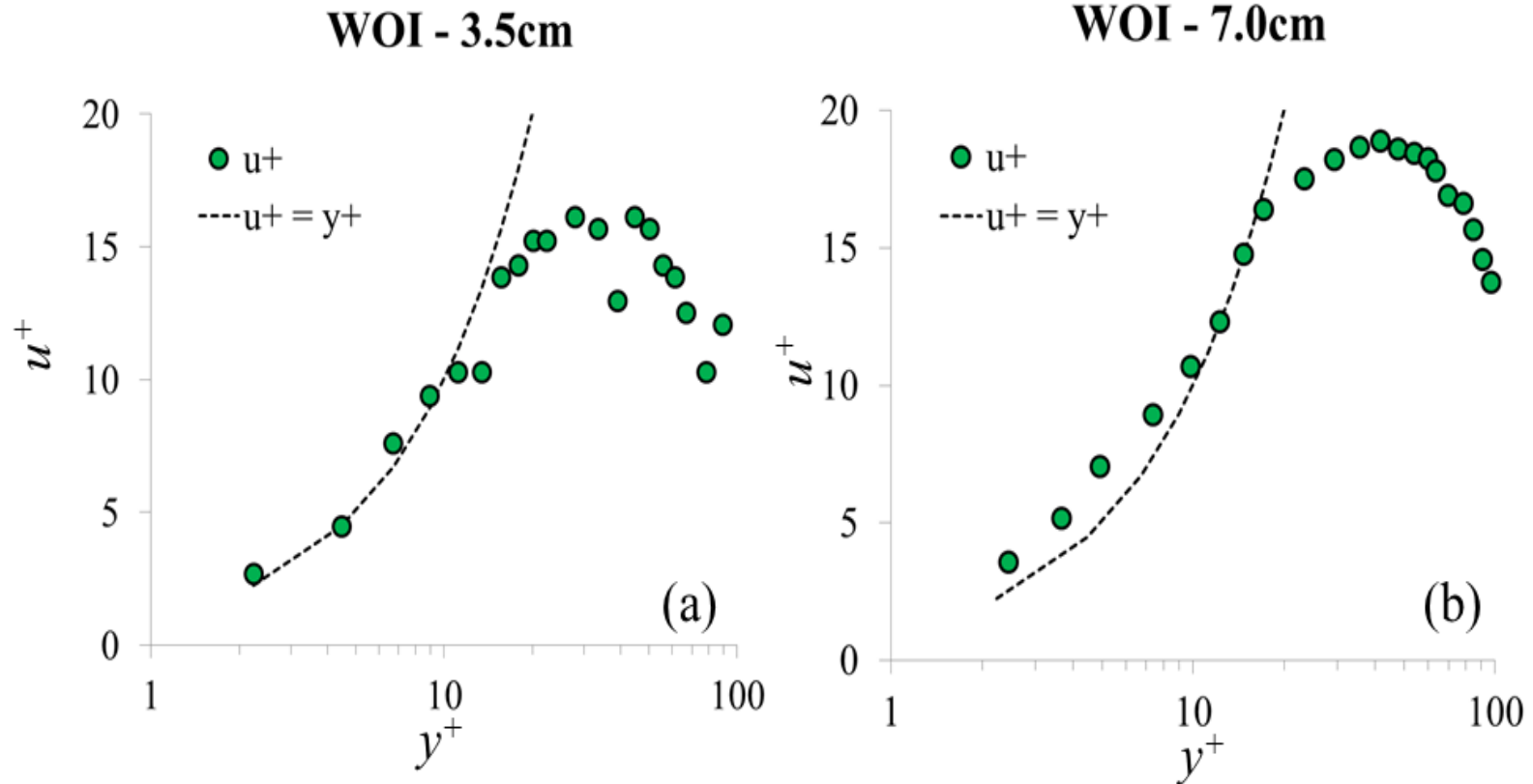


7 cm from the SEN

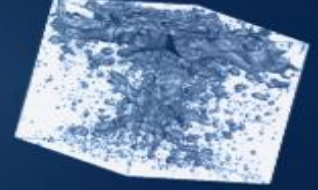


## Simulation of the Water-oil CC model

- Velocity profile near the interface

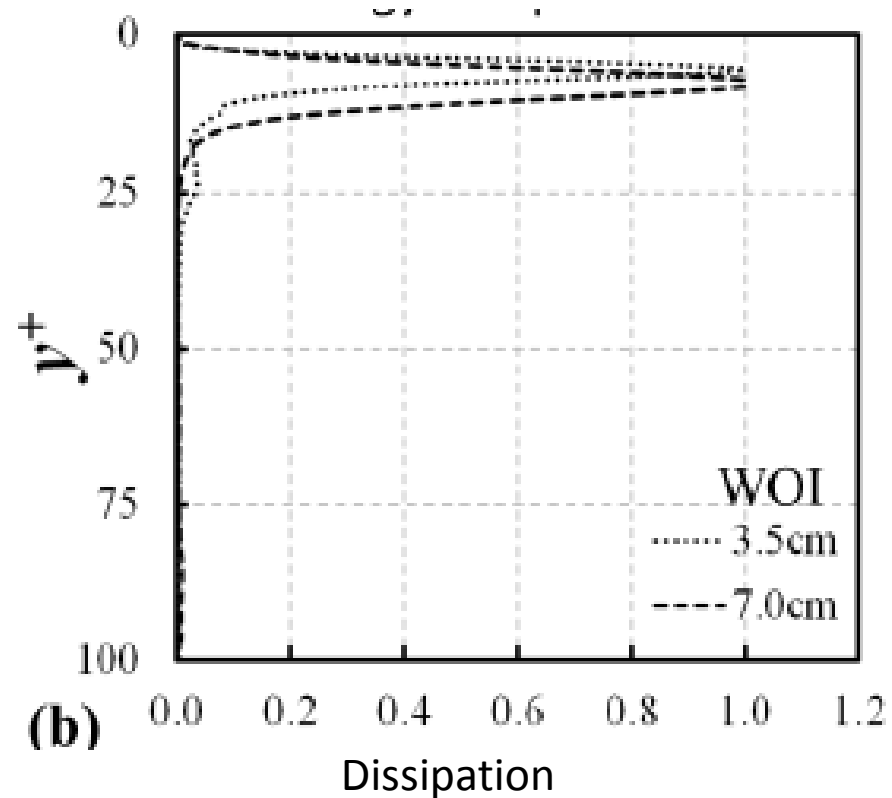
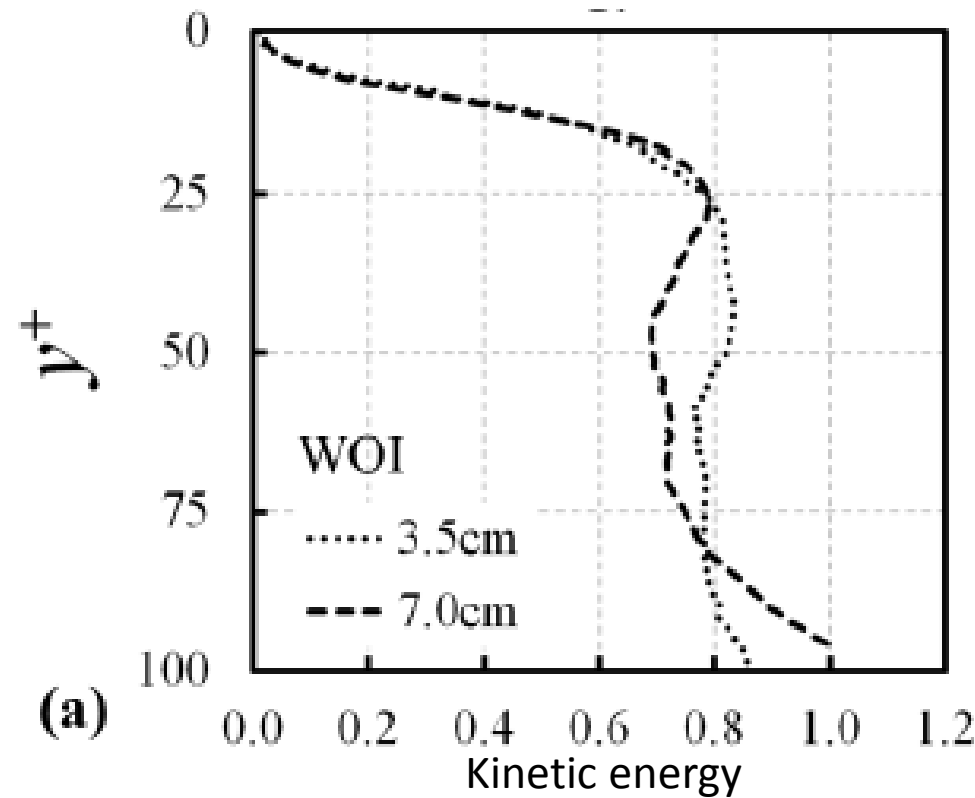


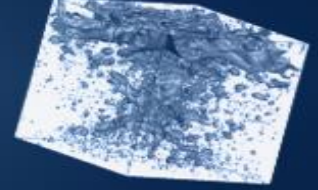




## Simulation of the Water-Oil CC model

- Kinetic energy and Dissipation





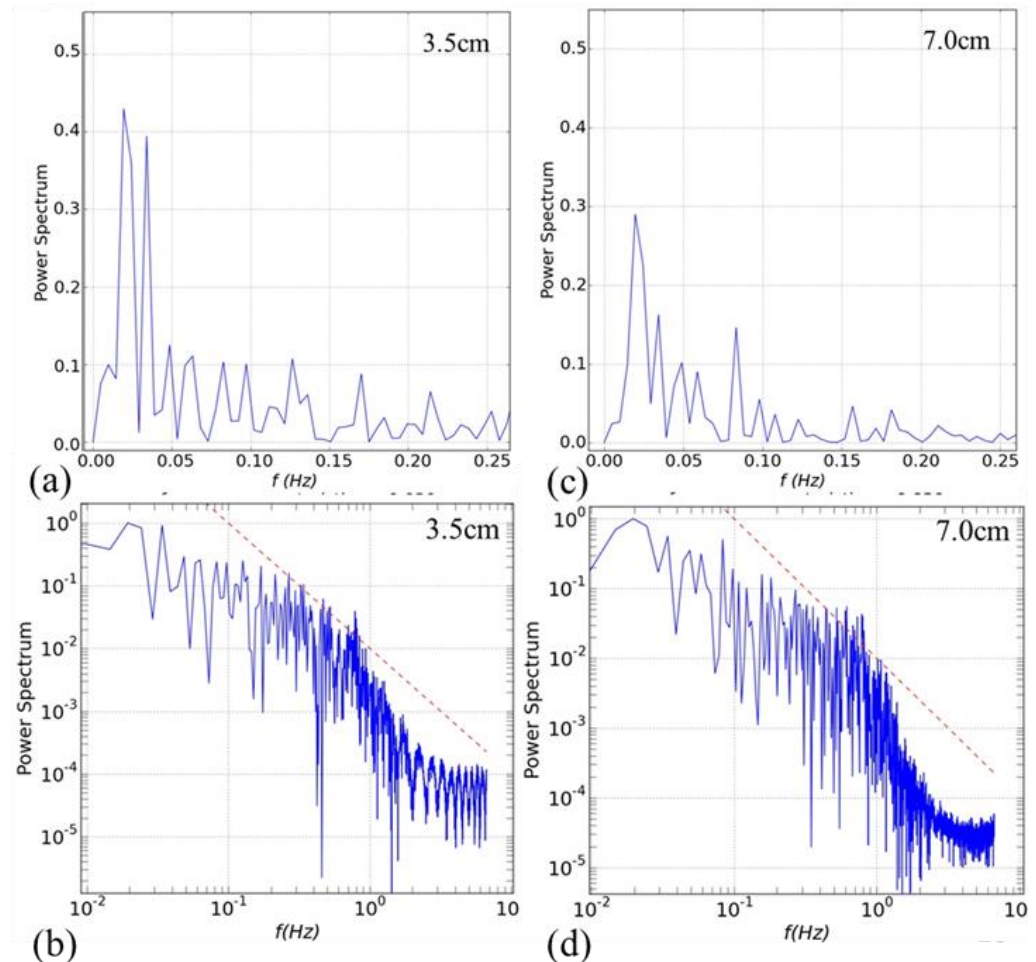
## Simulation of the Water-Oil CC model

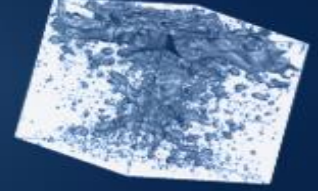
- Spectrum of the interface displacement in the WO CC simulation**

The simulated results indicate a characteristic period of the interface waves of about 50 s.

Good agreement is found between experiments and calculations concerning interface motion description.

The characterization of the wave peak has direct implication on mass transfer modeling [McCready *et al.*, AIChE Journal, 1986]





## Mass transfer at liquid/liquid interfaces

- **Large Eddy Model (LEM)** of [S. Banerjee & S. MacIntyre, Santa Barbara: Department of Chemical Engineering - University of California, 1998]

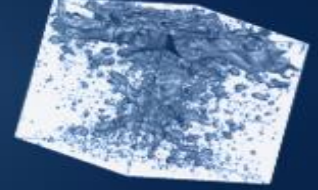
$$k = 0.1u^*Sc^{-1/2}$$

Shearing velocity                      Schmidt number

- **Surface Divergence Model (SDM)** of [M. McCready et al. , AIChE Journal, 1986]

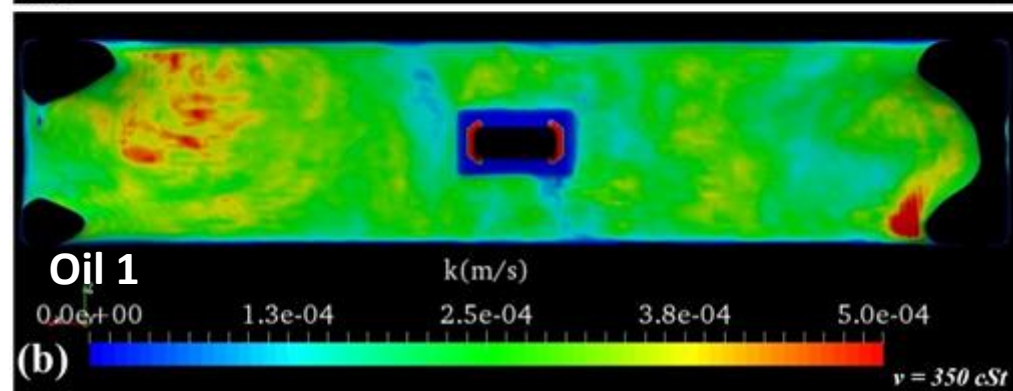
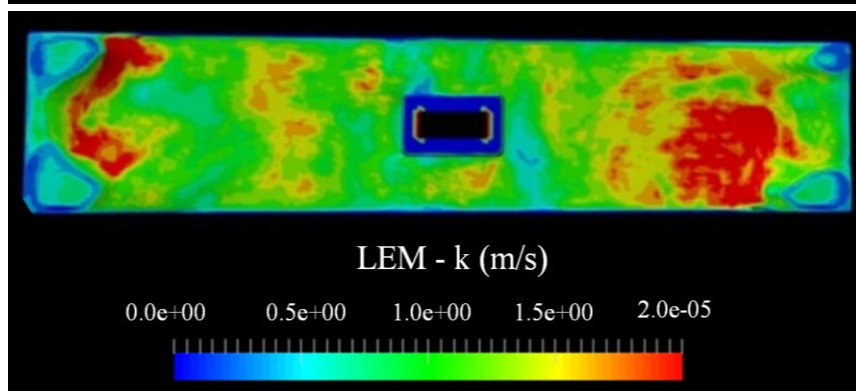
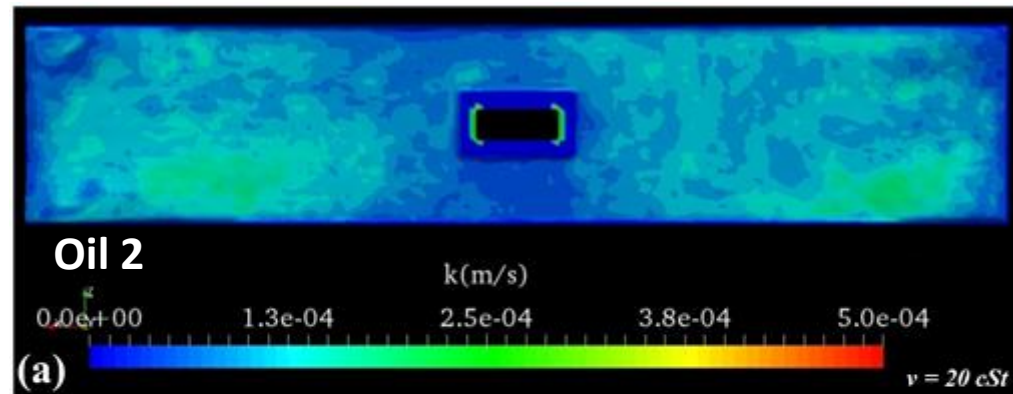
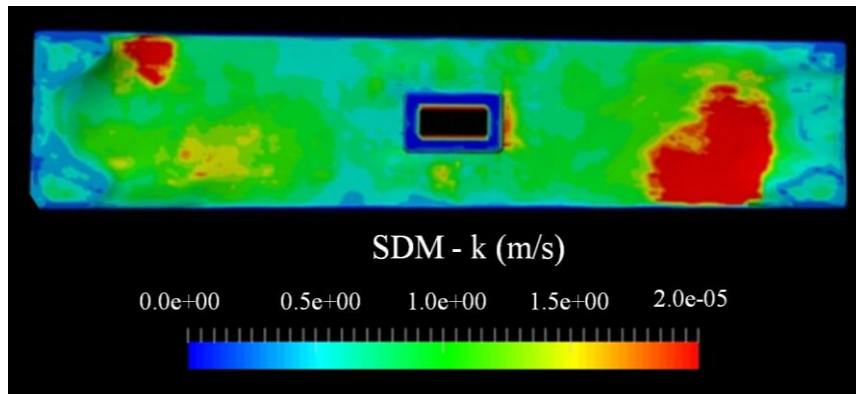
$$k = 0.71\sqrt{D\gamma'}$$

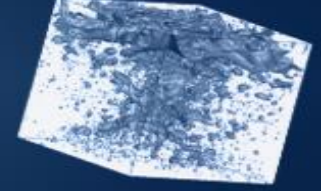
Mass diffusion coefficient                      Fluctuation of surface divergence



## Mass transfer at liquid/liquid interfaces

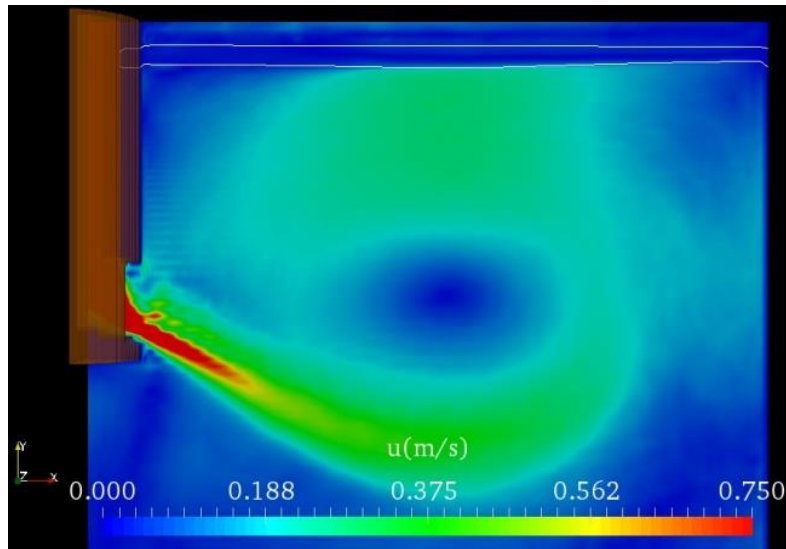
- Mass transfers obtained based on models (LEM, SDM) and simulated values (surface divergence, shearing velocity)



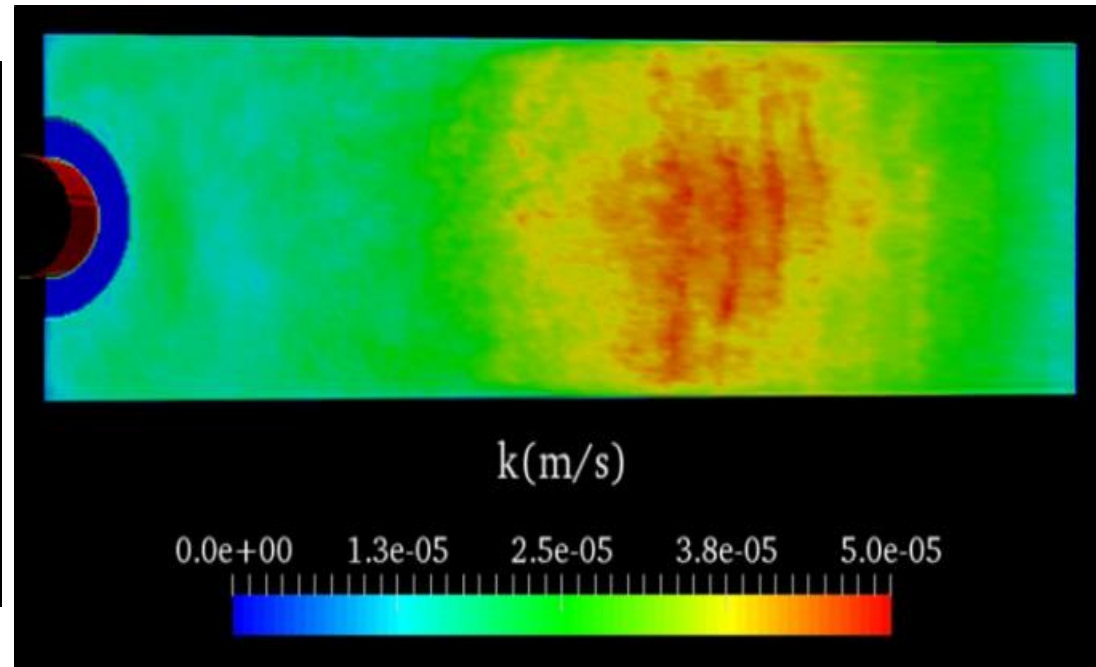


## Mass transfer at liquid/liquid interfaces

- Mass transfers obtained based on SDM model for a steel/slag interface

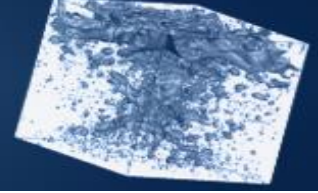


Average velocity



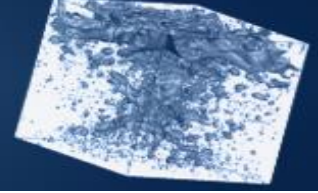
Average mass transfer coefficient

**Heterogeneous character of the mass transfer at the steel/slag interface**



## Conclusions - perspectives

- For the first time, a two-phase VOF-LES simulation tool has been successfully validated against a Water-oil CC model
- LDA experiments of CC model have been realized and allowed deep validation of simulations and understanding of physics
- Mass transfer coefficients have been calculated thanks to different models (LEM,SDM) with equivalent results
- Future works concern the use of mass transfer results in large scale process codes (CECSI)
- Implementation of LES two-phase subgrid terms with ADM approaches [Vincent et al. Comput. Fluids, 2016]



## Thank you for your attention

Instantaneous velocity

Dissipation

