20010 NETL Multiphase Flow Science Workshop
May 4-6, 2010

Modelling and Simulation of Unsteady Reactive Fluid-Particle Multiphase Flows

M. Abbas, A. Ozel, JF Parmentier,
R. Ansard, A. Konan, B. Metay,
E. Climent, P. Fede, H. Neau, O. Simonin

Institut de Mécanique des Fluides de Toulouse
Groupe Particules, Spray et Combustion
UMR CNRS/INPT/UPS
Université de Toulouse

General context

Institut de Mécanique des Fluides de Toulouse (IMFT)

Unité Mixte de Recherche CNRS / INPT / UPS

About 200 peoples (70 PhD, 20 Post-Doc)

Main research topics : instabilities and transition, heterogeneous media, environmental flows, multiphase and reactive flows (→ Particles, Spray and Combustion Group),

Methodology : theoretical, experimental and numerical approaches

Application domains : transport & energy (45%), process engineering (30%), environment (15%), life sciences (10 %)

FERMaT

Institut Fédératif de Recherche CNRS / INPT / UPS / INSA

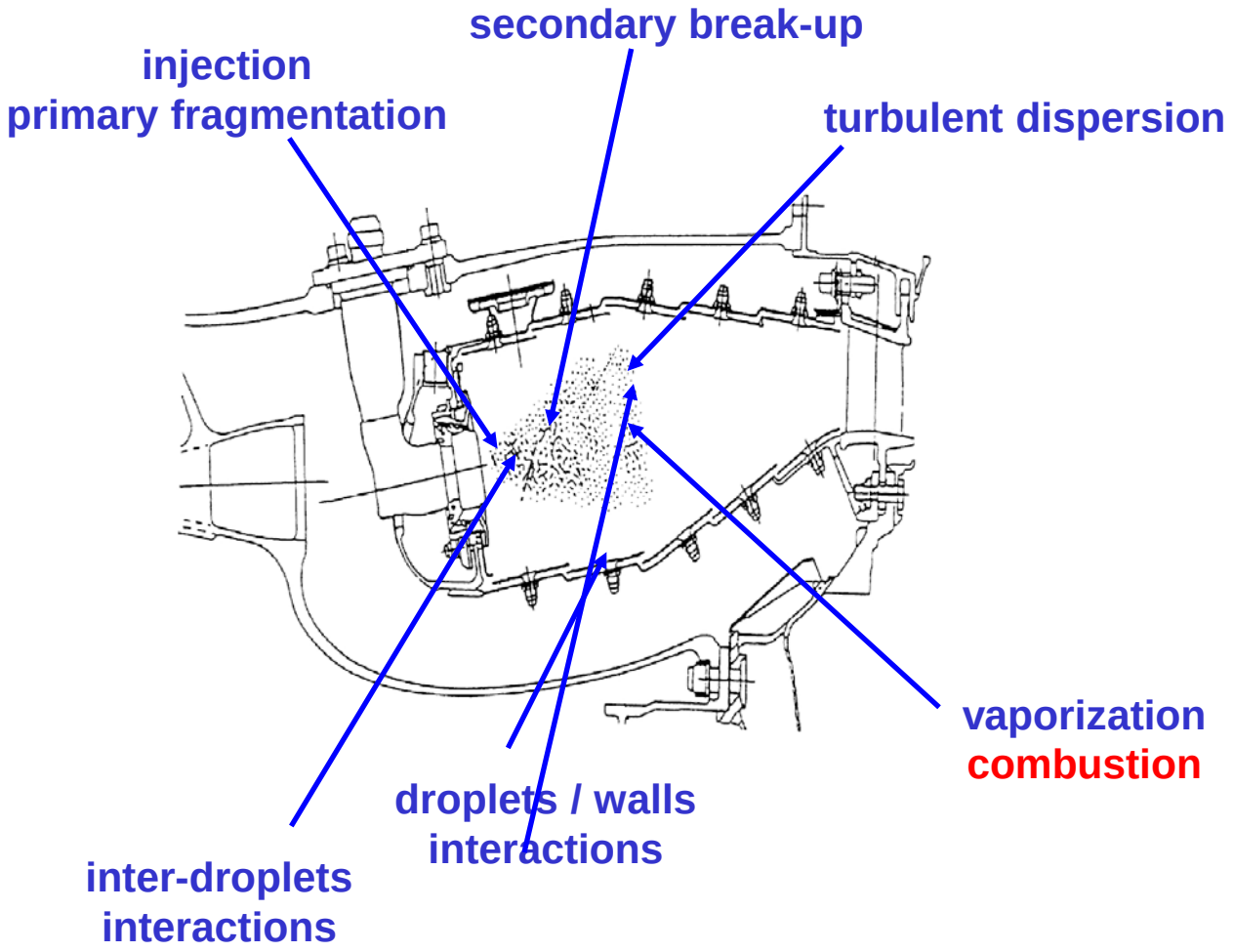
Collaboration projects between 6 laboratories (Toulouse) :

LGC – IMFT – LISBP – LAPLACE – LAAS - CIRIMAT

About 160 permanent researchers

Multidisciplinary research projects : flow, energy, process engineering, materials

Research objectives and methods



A paradigm: the aircraft combustion chamber

Research objectives and methods

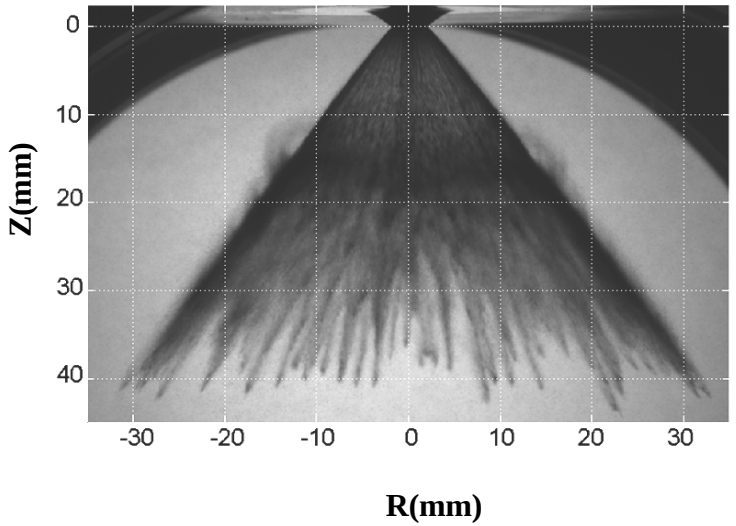
- Explore and model local interactions and medium scale behavior in reactive and/or multiphase flows with dispersed phases of solid particles or droplets by using experiments and direct numerical simulations.

- Develop numerical modeling approaches for full-scale predictions of reactive particulate multiphase flows in the general frame of kinetic theory of particulate flows:
    - fluid-particle joint probability density function (PDF) equation,
    - "n-fluid" (or moment) and stochastic Lagrangian (or Monte Carlo) methods coupled with RANS fluid equations,
    - Euler-Euler and Euler-Lagrange large-eddy simulation (LES) approaches

- Full scale prediction of industrial (and environmental) flows:
    + Evaluation of available numerical modeling approaches (comparison with experimental results),
    + Optimization and scale-up of existing processes,
    + Support for development of new processes.

Industrial research projects

+ Ground transportation:
  - Injection in IC engine
  - Droplet deposition

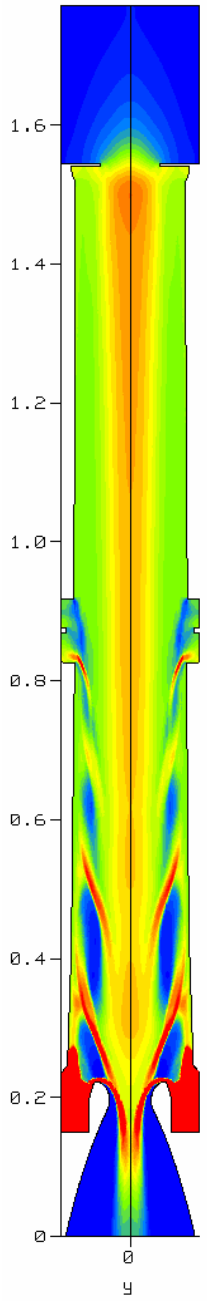


Gazoline spray HP (200 bars)

Industrial research projects

+ Ground transportation:
    - Injection in IC engine
    - Droplet deposition

+ Air and space transportation:
    - Aircraft turbines
    - Cryogenic engine
    - Solid fuel rocket booster



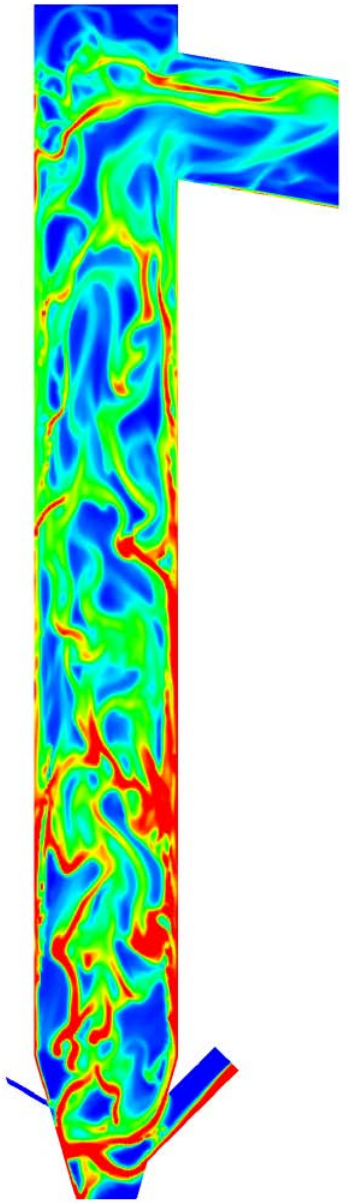
Al_2O_3 droplet concentration field in solid fuel rocket combustion chamber

Industrial research projects

+ Ground transportation:
    - Injection in IC engine
    - Droplet deposition

+ Air and space transportation:
    - Aircraft turbines
    - Cryogenic engine
    - Solid fuel rocket booster

+ Energy and safety:
    - Particle transport and deposition
    - Spray into the enclosure of a nuclear reactor
    - Coal boiler for CO2 capture: "chemical looping"



MeOx concentration field. NEPTUNE_CFD bi-solid prediction of the circulating fluidized bed coal combution reactor (chemical looping fuel reactor)

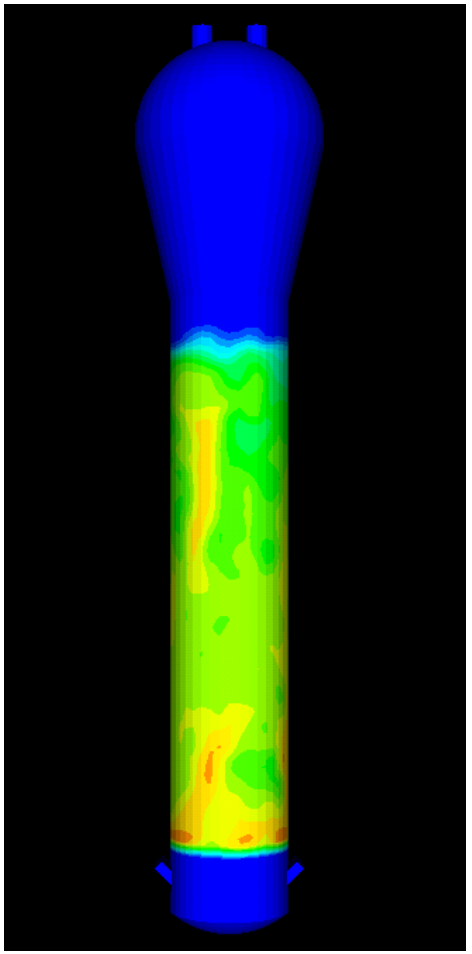
Industrial research projects

+ Ground transportation:
  - Injection in IC engine
  - Droplet deposition

+ Air and space transportation:
  - Aircraft turbines
  - Cryogenic engine
  - Solid fuel rocket booster

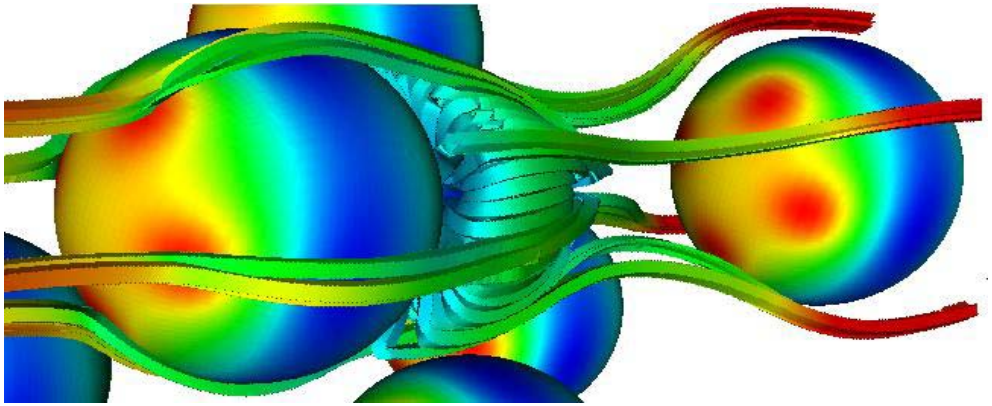
+ Energy and safety:
  - Particle transport and deposition
  - Spray into the enclosure of a nuclear reactor
  - Coal boiler for CO2 capture: "chemical looping"

+ Process engineering:
  - Fluid catalytic cracking column
  - Fluidized bed chemical reactor (UF_4 fluoration, Zirconium chloration, olefin polymerization)
  - Glass melting furnace
  - Hydrocyclone,
  - …



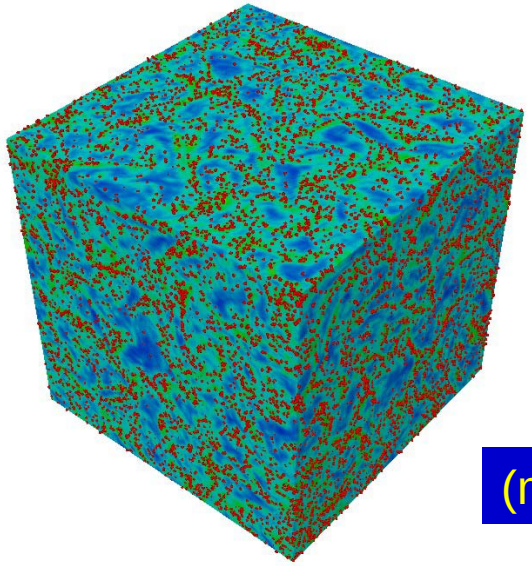
Solide particle concentration field.
NEPTUNE_CFD 3D unsteady prediction of industrial olefin polymerization reactor

Multi-scale numerical approach



(micro)

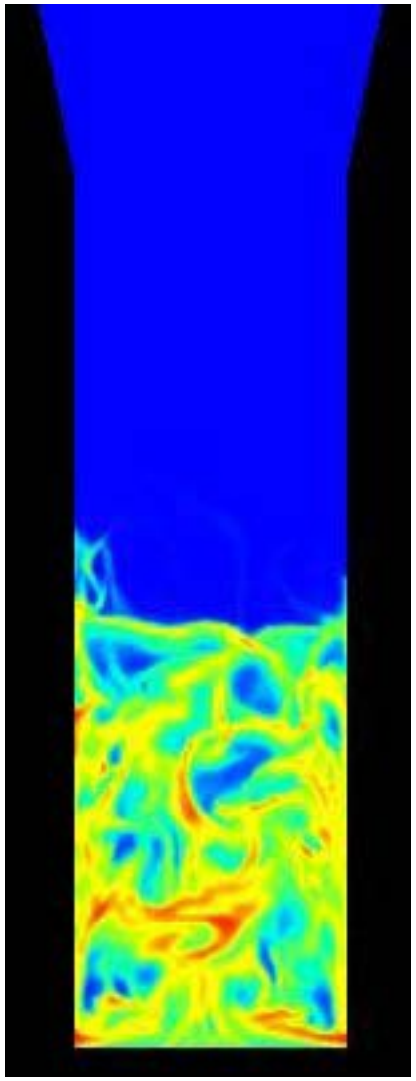
DNS in a particle array
(~1 mm)



(meso)

LES+DPS of particulate flow with a very large number of particles (~10 cm)

(macro)



N-fluid simulation at the Industrial scale (~10 m)

Numerical Tools

- VOF type method: Thétis (TREFLE, Bordeaux)

- Eulerian-Lagrangian approaches:
  + "DNS"-DPS: JADIM (Interface-IMFT), NTMIX (CERFACS)
  + LES-DPS: JADIM (Interface-IMFT), AVBP (CERFACS)

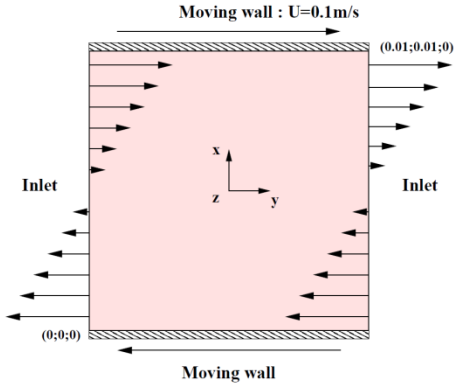
- n-Eulerian statistical model:
  + NEPTUNE_CFD (EDF R&D) → dense particulate flows (parallel multi-phase code, implicit, unstructured VF), NEPTUNE project (CEA, EDF, IRSN and AREVA-NP)
  + AVBP (CERFACS) → dilute droplet flows with turbulent combustion

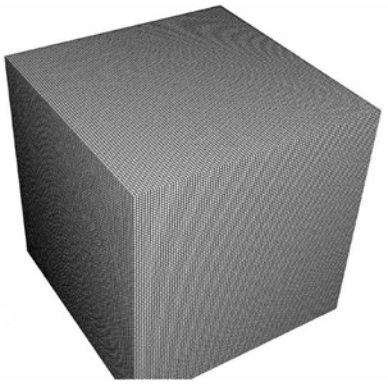
Numerical Tools

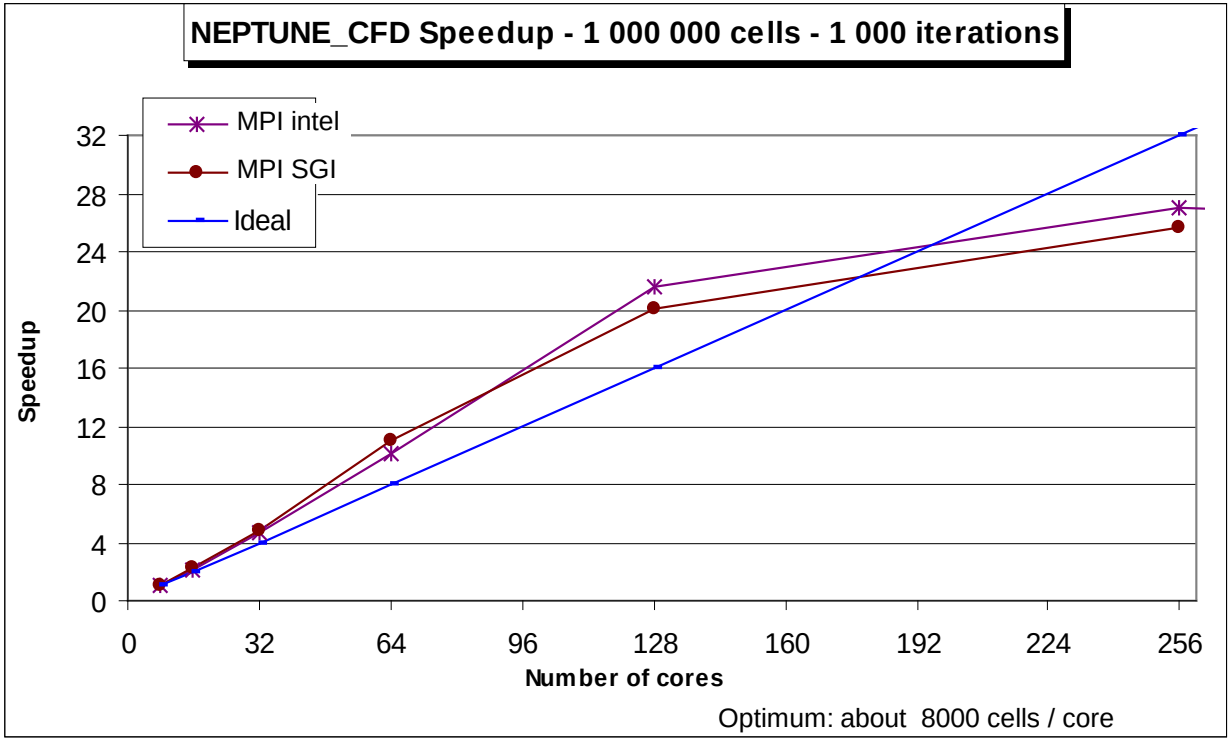
NEPTUNE_CFD computation efficiency:

Test case of a simple granular shear flow

Neau, Laviéville, Simonin, ICMF 2010 - Tampa







Outlines

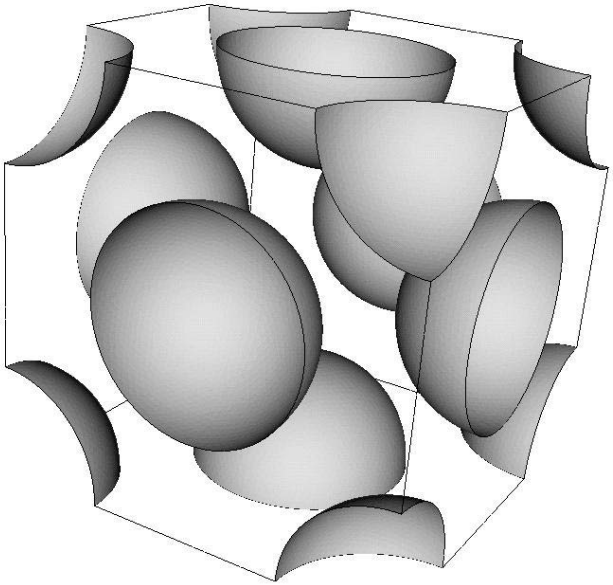
- Direct numerical simulation of fluid-particle interactions
    + Flow simulation in fixed array of solid particles
    + VOF type simulation of a liquid-solid-fluidized bed

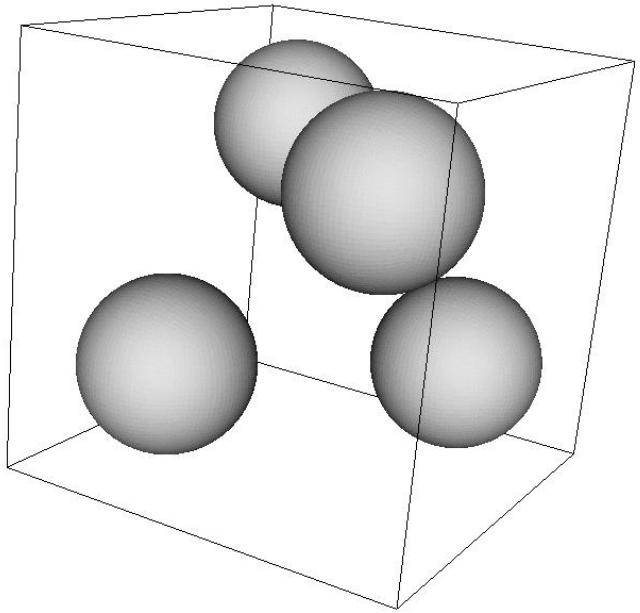
- Kinetic theory of dense particulate flows
    + Self-diffusion of particles with finite inertia
    + Polydisperse moment approach

- n-Eulerian modeling approach
    + « Coarse-grid » model development
    + Experimental validation and industrial application

- Conclusion

Direct numerical simulation of fluid-particle interactions

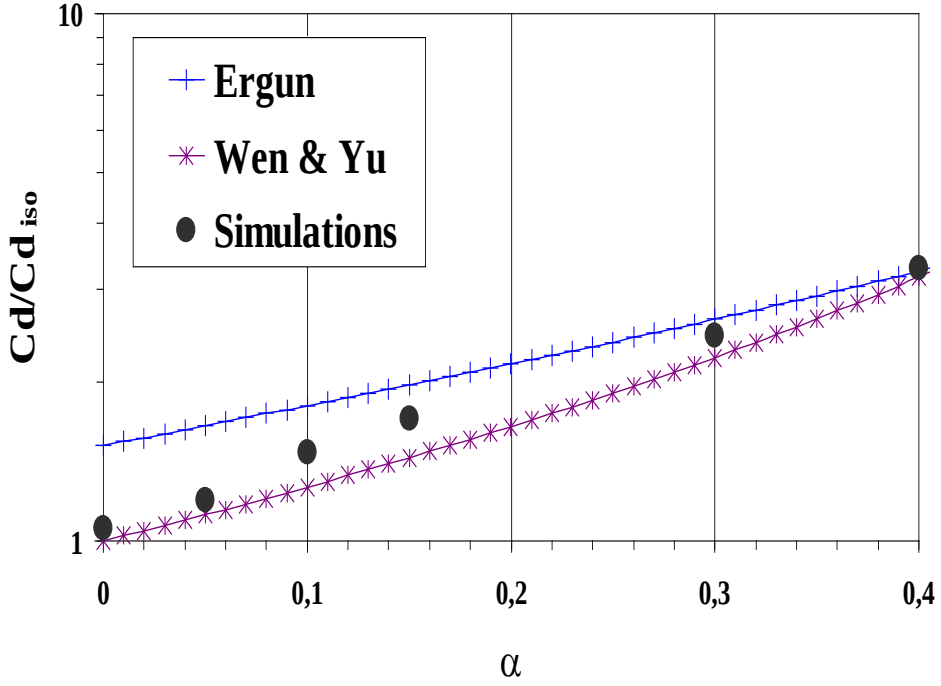




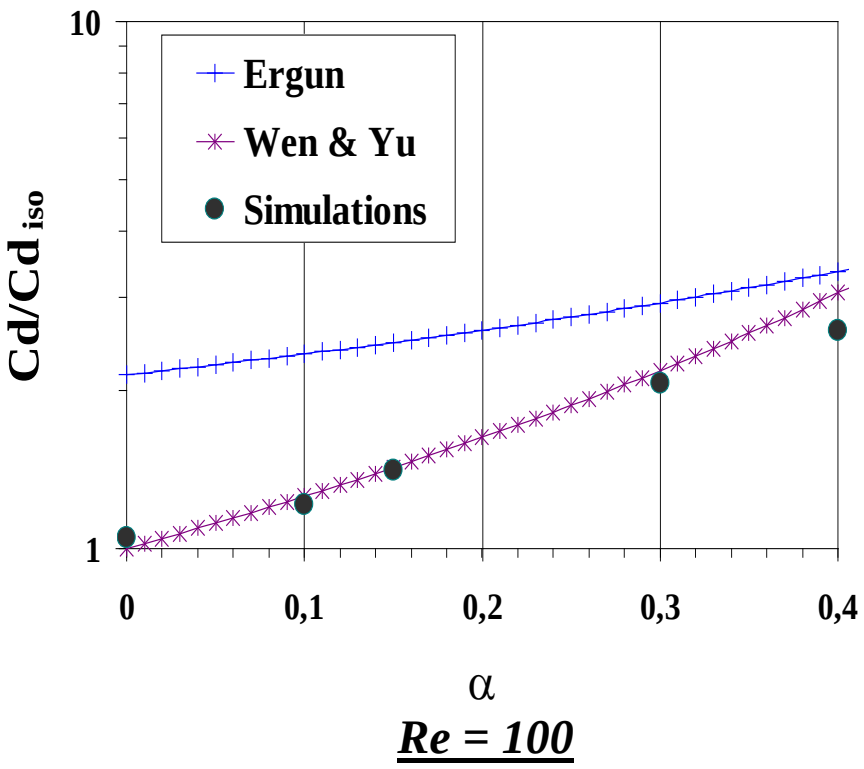
- **Regular arrays of equal sized particles (cubic face centered arrays)**
- **$50 \leq Re \leq 300$; $0 \leq \alpha_s \leq 0.60$ (α_s solid volume fraction)**

AVBP computation of momentum and heat transfert coefficients in a regular array of fixed reactive particles ($Re = V_r\, d_p / \nu_f$).

Direct numerical simulation of fluid-particle interactions



Re = 50



Re = 100

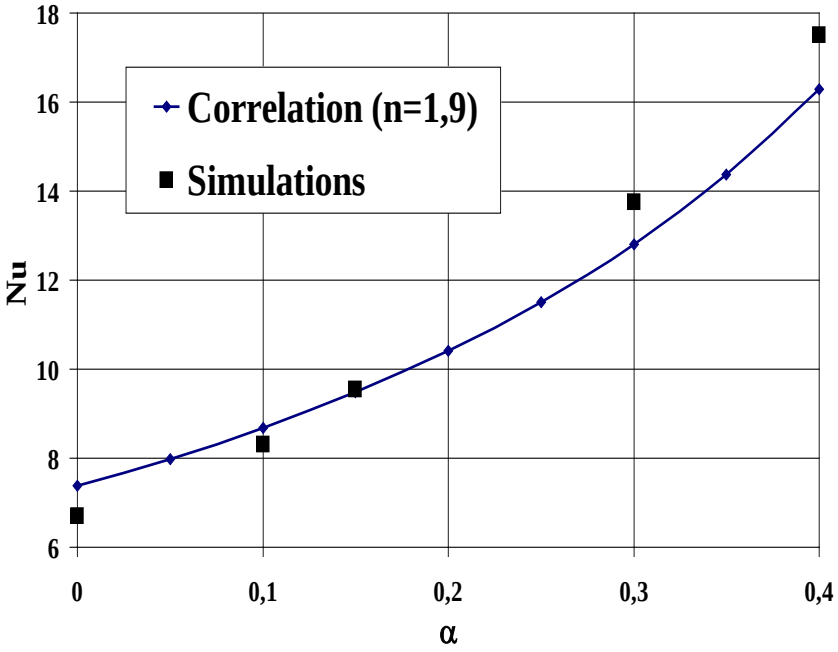
AVBP (CERFACS) computation of drag coefficient in a regular array of fixed particles (*Re* = $V_r\, d_p / \nu_f$).

Proposed drag coefficient correlation:

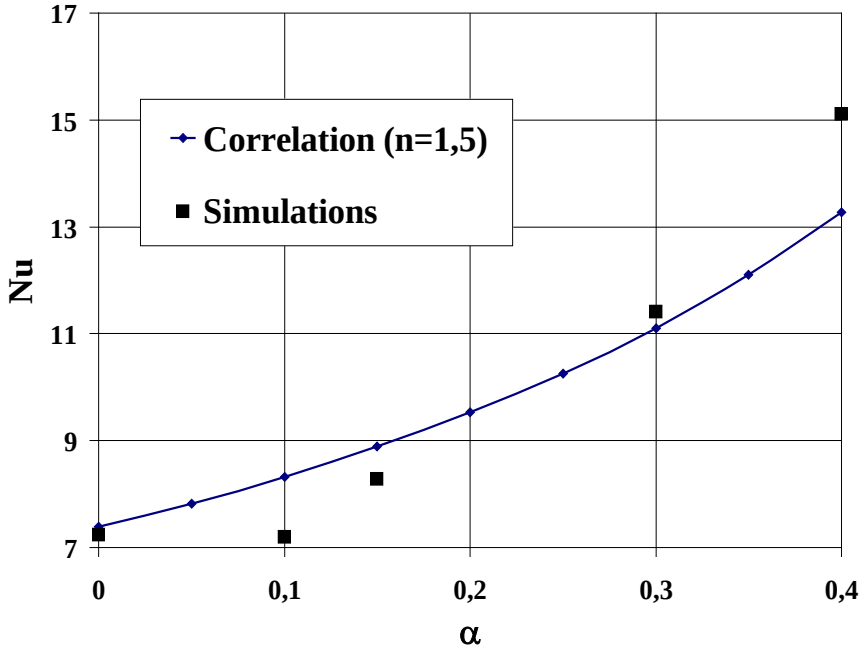
$$Cd = Cd_{W\&Y} \qquad \alpha_p \le 0.3$$

$$Cd = \min\left[Cd_{W\&Y}, Cd_{Erg}\right] \qquad \alpha_p > 0.3$$

Direct numerical simulation of fluid-particle interactions



Re=100 ; Pr=0.72



Re=100 ; Pr=2

AVBP (CERFACS) computation of heat transfert coefficient in a regular array of fixed reactive particles (*Re = V_r d_p / ν_f*).

Proposed Nusselt correlation: $Nu = \alpha_f^{-n}(2 + 0.6\,\mathrm{Re}^{0.5}\,\mathrm{Pr}^{0.33})$

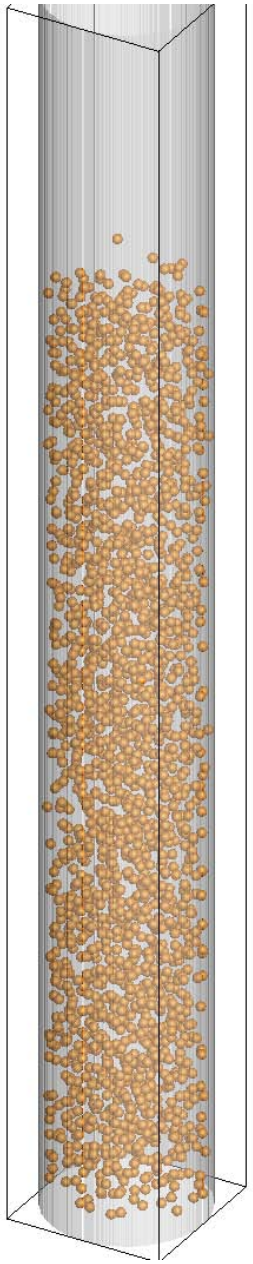
Direct numerical simulation of fluid-particle interactions

+ Perspectives:

- Simulation of heterogeneous combustion in a regular array of solid particle

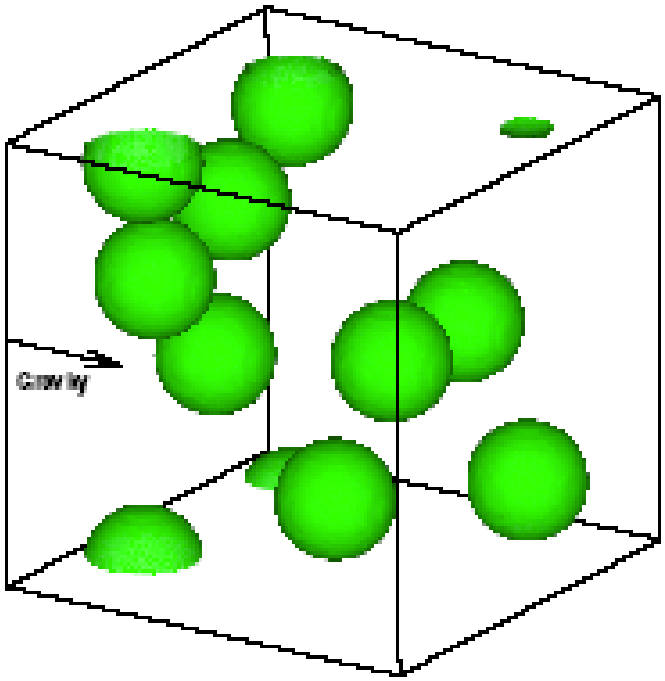
- Full direct simulation of liquid solid fluidized beds

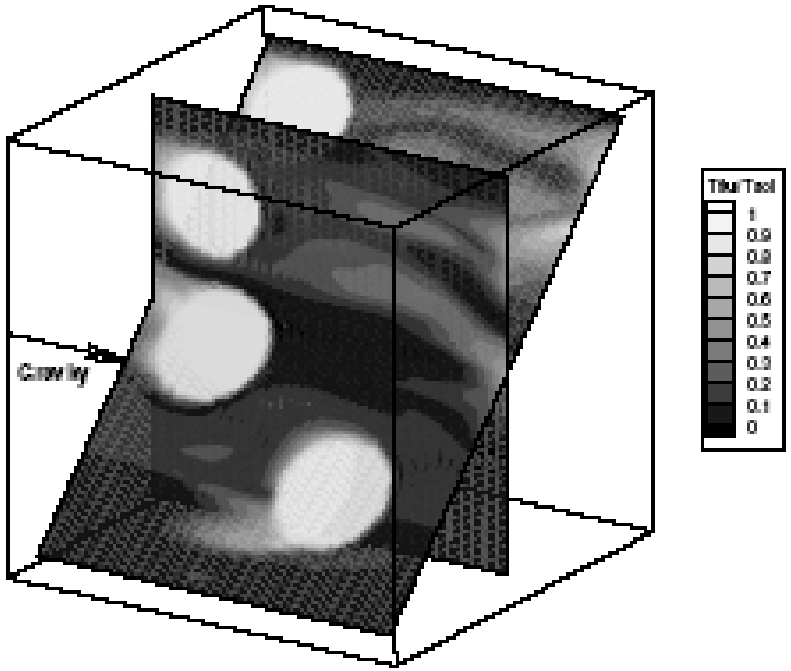
→ comparison with experimental results (LGC, Toulouse)



Vertical column with diameter equal to 80 *mm*
2133 glass particle with diameter equal to 6 *mm* and density 2230 kg/m^3
The fluid is a solution of potassium thiocynate KSCN with a density equal to 1400 kg/m^3 and a kinematic viscosity equal to $3.8\ 10^{-3}$ *Pa.s*.
Fluidisation velocity equal to 0.12 m/s

Direct numerical simulation of fluid-particle interactions

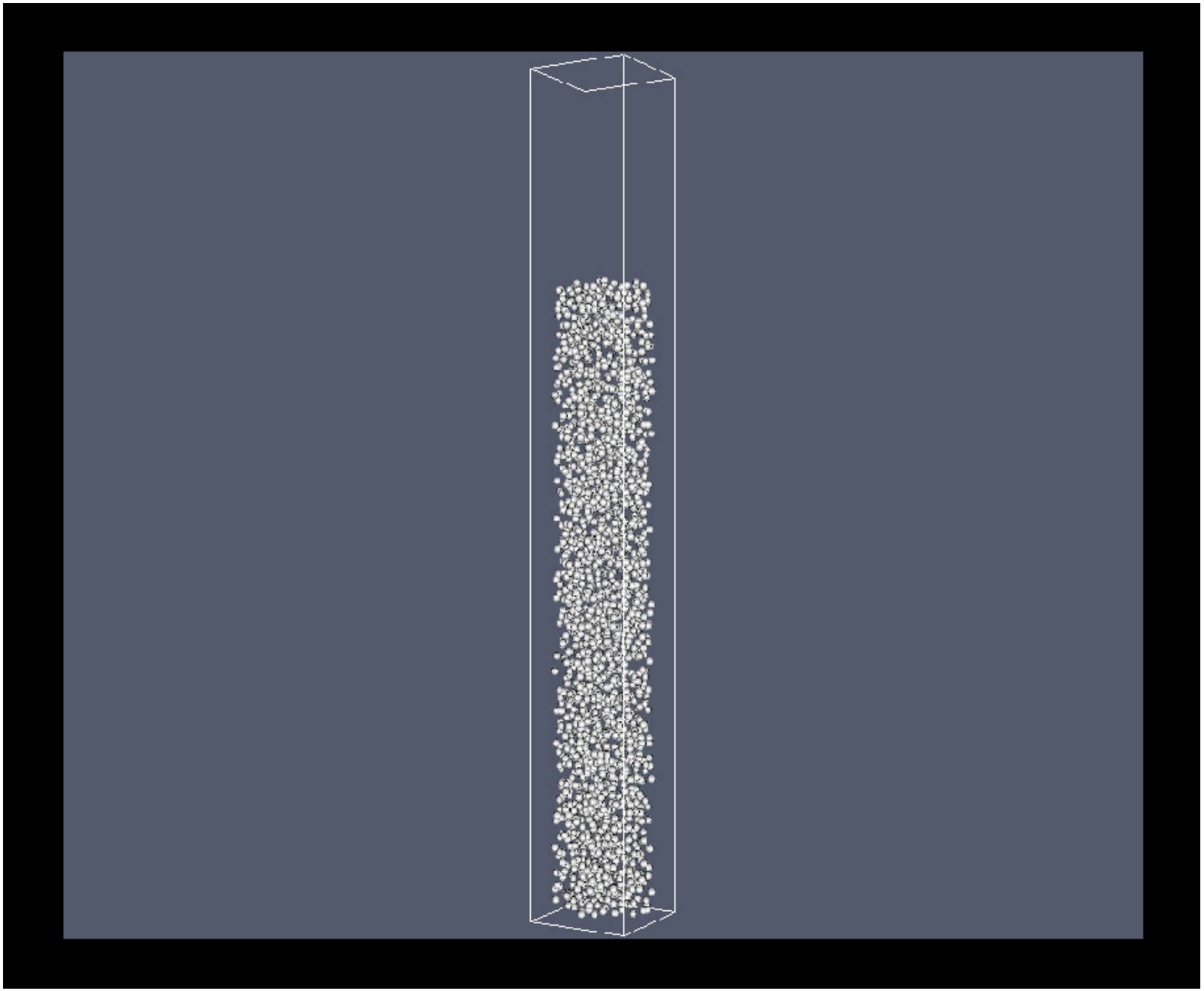




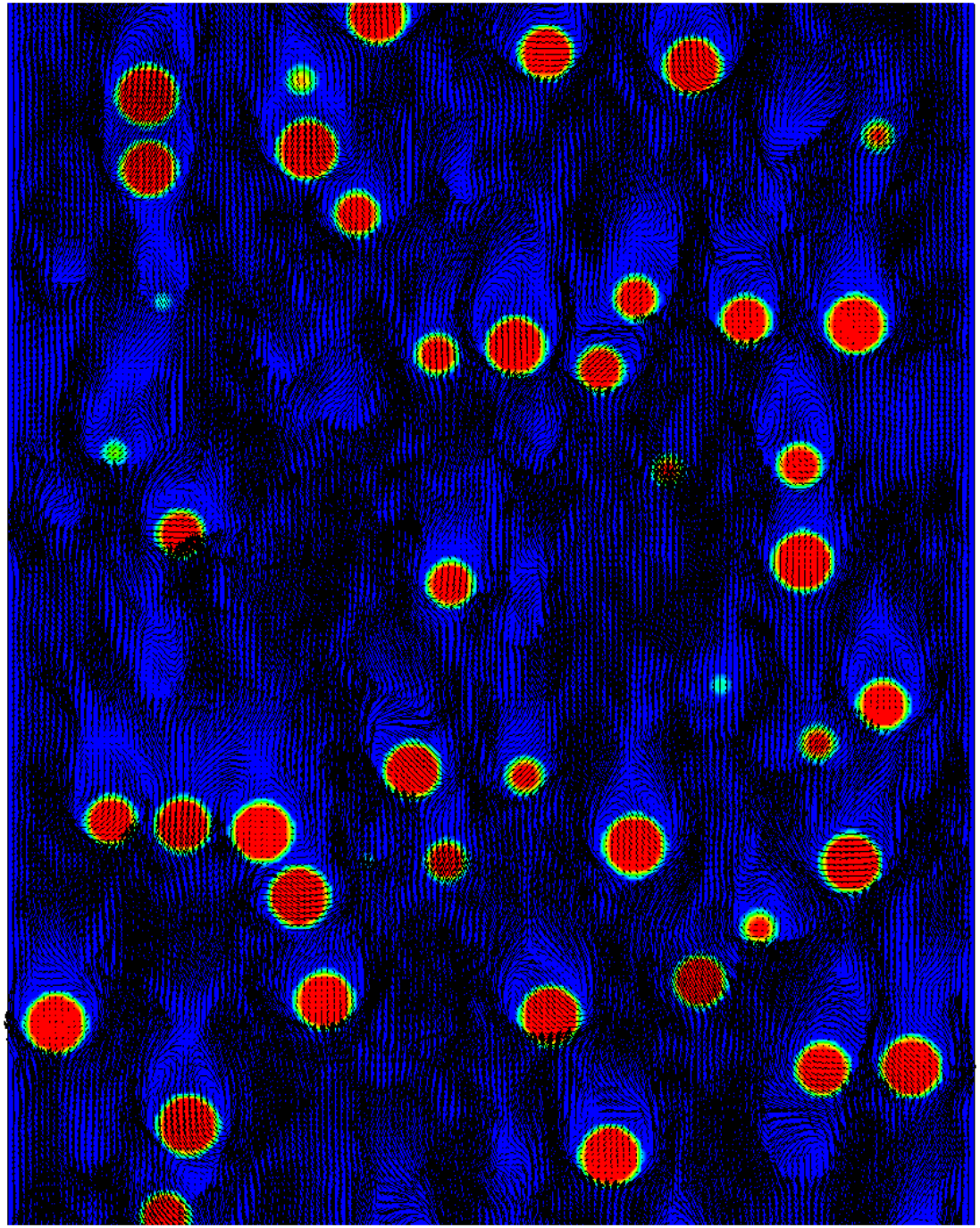
THETIS computation of fluidized heated particles using single-fluid simulation with variable physical properties (density, viscosity, heat, diffusivity).
Interface tracking based on phase distribution transport equation : VOF methodology.

LABORATOIRE INTERETABLISSEMENTS
TREFLE
UMR CNRS 85 08

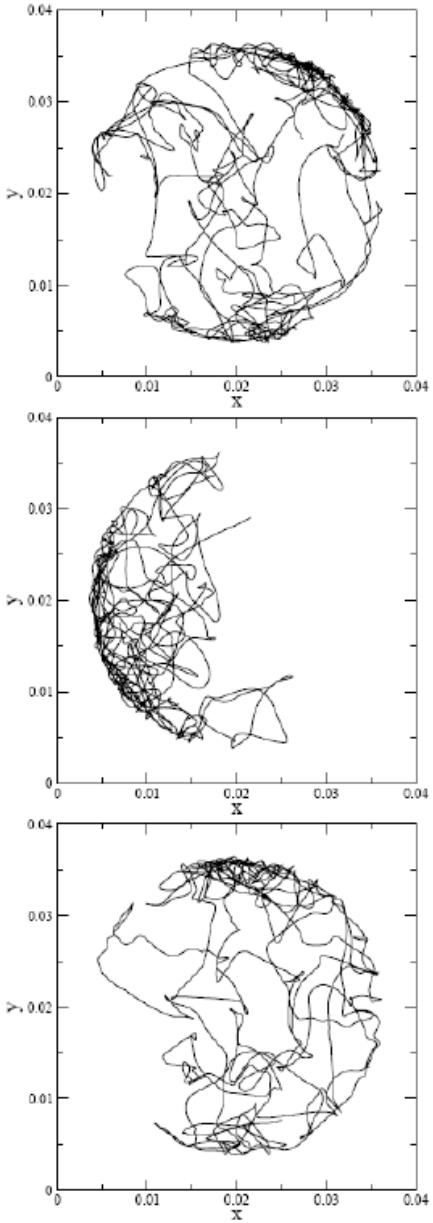
IMFT



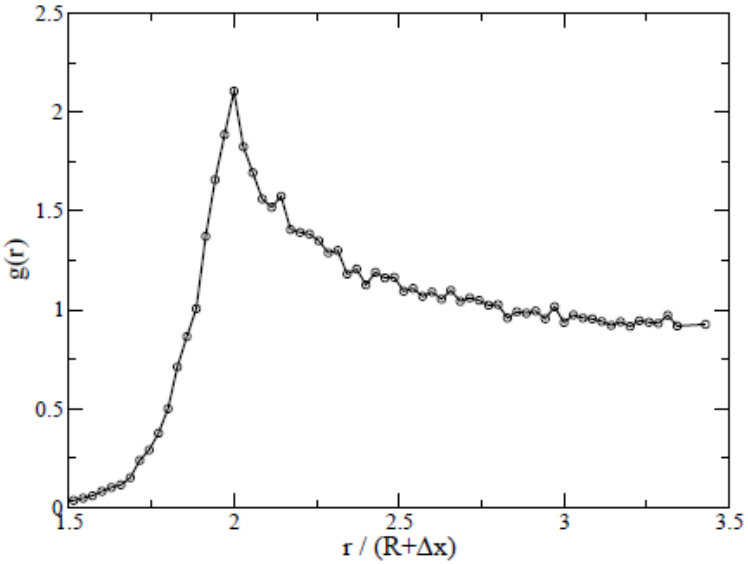
*Thétis VOF type simulation of a liquid-solid fluidized bed (150*150*800). Computation of the LGC experiment (ONERA / TREFLE / IMFT): bed diameter, 80 mm; particle diameter, 6 mm (N_p= 2133).*



Direct numerical simulation of fluid-particle interactions



Examples of time evolution of horizontal coordinates of three different particles - trajectories are observed from the top of the fluidized bed.



Pair distribution function $g(r)$ according to dimensionless radius $r/(R + \Delta x)$.

Outlines

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- Kinetic theory of dense particulate flows
    + Self-diffusion of particles with finite inertia
    + Polydisperse moment approach

- n-Eulerian modeling approach
    + « Coarse-grid » model development
    + Experimental validation and industrial application

- Conclusion

Kinetic theory of dense particulate flows

Methodology

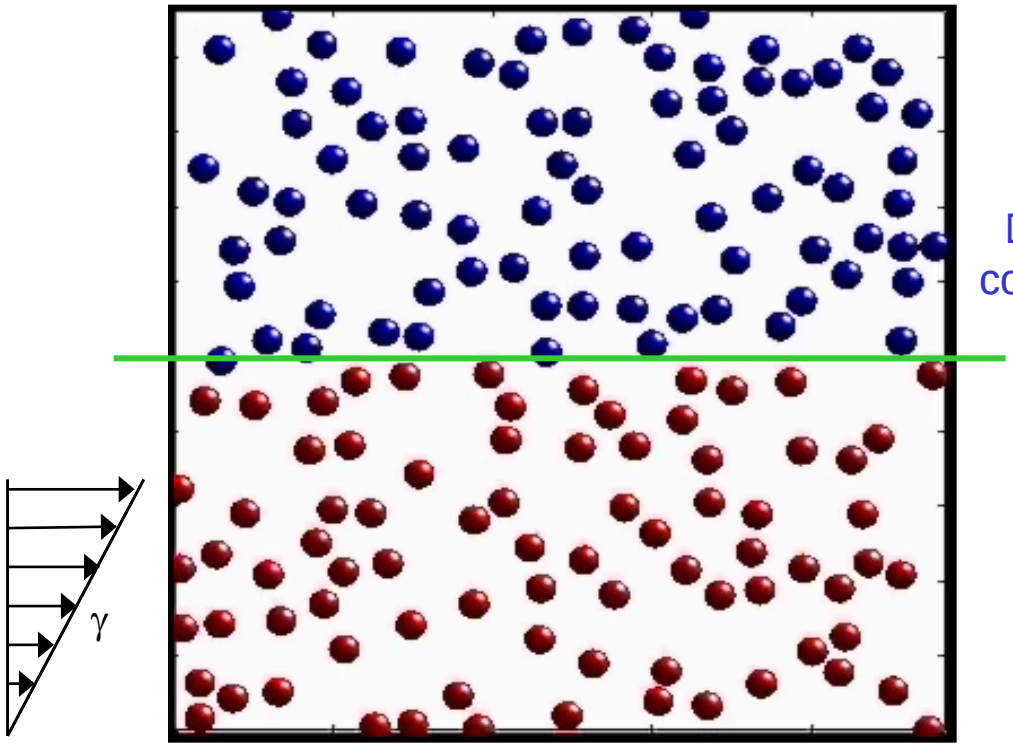
Closure of the kinetic transport equation on the single particle PDF based on a Lagrangian modelling of particle-fluid, particle-particle and particle-wall interactions.

Derivation of the moment transport equations (concentration, velocity, temperature, fluctuating motion kinetic energy, kinetic stresses…) and the transport properties (viscosity, diffusivity).

Validation from "*Euler-Lagrange numerical experiments*"

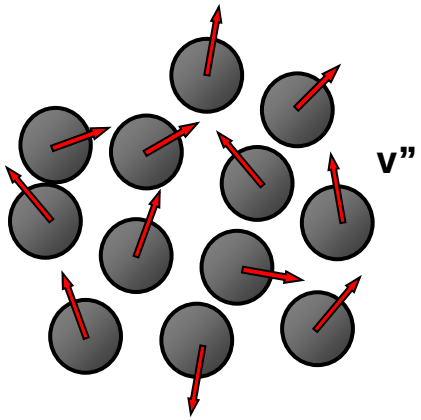
→ Implementation in NEPTUNE_CFD and comparaison of model predictions with experimental measurements (laboratory, pilot and industrial scales).

Kinetic theory of dense particulate flows



Drag + collisions

⇨ **Particle agitation**



⇨ Chaotic suspension evolution

⇨ Loss of velocity correlation

⇩ **Self-diffusion**

Objectives

- Understand the physics for variable particle St ($St = \tau_p \gamma$)
- Suspension prediction using an adapted theory
- Suggest a prediction for Self-Diffusion

Kinetic theory of dense particulate flows

Kinetic theory adapted to moderate particle inertia

- Transport of f (**c**,**x**,t) (Boltzmann equation)

$$\frac{\partial f}{\partial t}+\frac{\partial}{\partial x_i}\left(c_i f\right)+\frac{\partial}{\partial c_i}\left(\frac{c_i - u_i}{\tau_p} f\right)=\frac{\partial_c f}{\partial t}$$

Variation in f | Drag contribution | Collision contribution

{c, x}: velocity and position phase spaces

f(c,x): velocity distribution function

Two-particle velocity distribution function modeling
Jenkins & Richman (1985)

- Kinetic stress equation

$$\rho_p \phi \frac{DT_{ij}}{Dt}+\frac{\partial}{\partial x_k}S_{ijk}=-\left[\sigma_{ki}\frac{\partial U_{p,j}}{\partial x_k}+\sigma_{kj}\frac{\partial U_{p,i}}{\partial x_k}\right]-\rho_p \phi \frac{2}{\tau_p}T_{ij}+\chi_{ij}$$

$$\sigma_{ij}=\sigma_{ij}^{kin}+\sigma_{ij}^{coll}$$

Momentum transfer

Collision effect

Kinetic stress

$$\sigma_{ij}^{kin}=\rho_p \phi T_{ij}$$

Collisional stress

$$\sigma_{ij}^{coll}=\theta_{ij}=\frac{2a}{\vartheta \times T_{sim}}\sum_{coll} m_p\left(j_i k_j\right)$$

Kinetic theory of dense particulate flows

χ_{ij} and θ_{ij}: Collision contribution

$f(\mathbf{c},\mathbf{x})$ must be known

Solution (Ignited theory)

Sangani et al. (JFM, 1996)
Boelle, Balzer & Simonin (ASME, 1995)

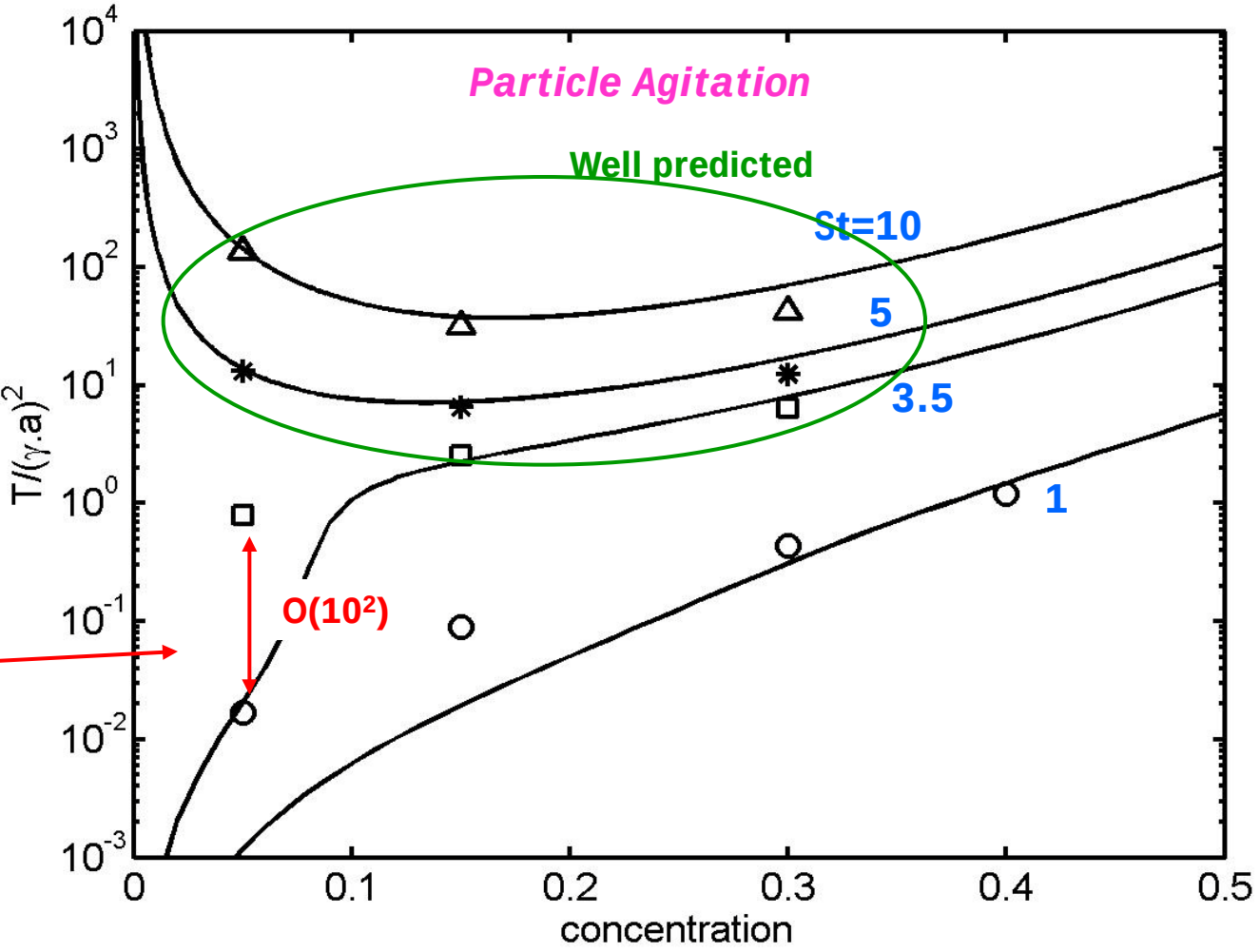
Deviated Maxwellian function

$$f(\mathbf{c},\mathbf{x}) = \left\{1 + \frac{T_{ij} - T\delta_{ij}}{2T}\frac{\partial^2}{\partial c_i \partial c_j}\right\} f_0(\mathbf{c},\mathbf{x})$$

Maxwellian

$$f_0(\mathbf{c},\mathbf{x}) = \frac{n}{(2\pi T)^{3/2}} \exp\left(-\frac{(\mathbf{c} - \mathbf{U}_p(\mathbf{x}))^2}{2T}\right)$$

Kinetic theory of dense particulate flows

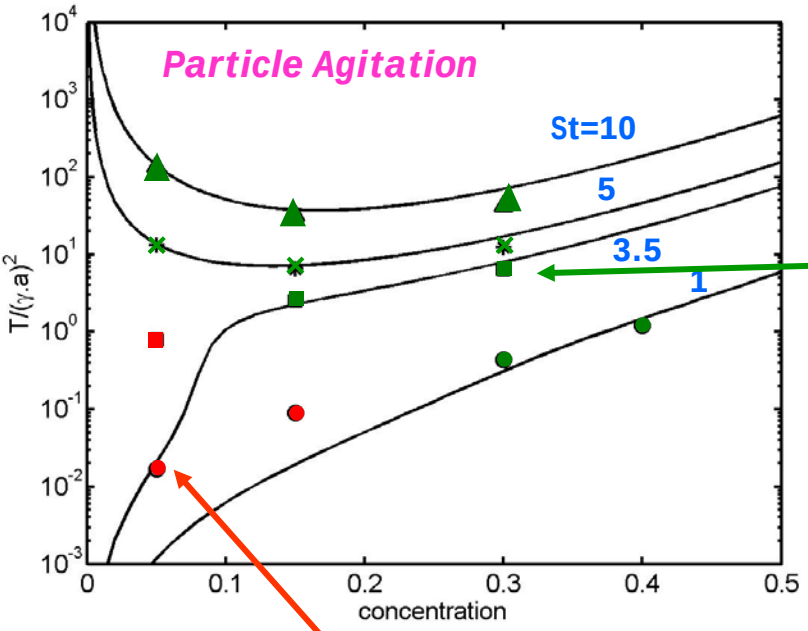


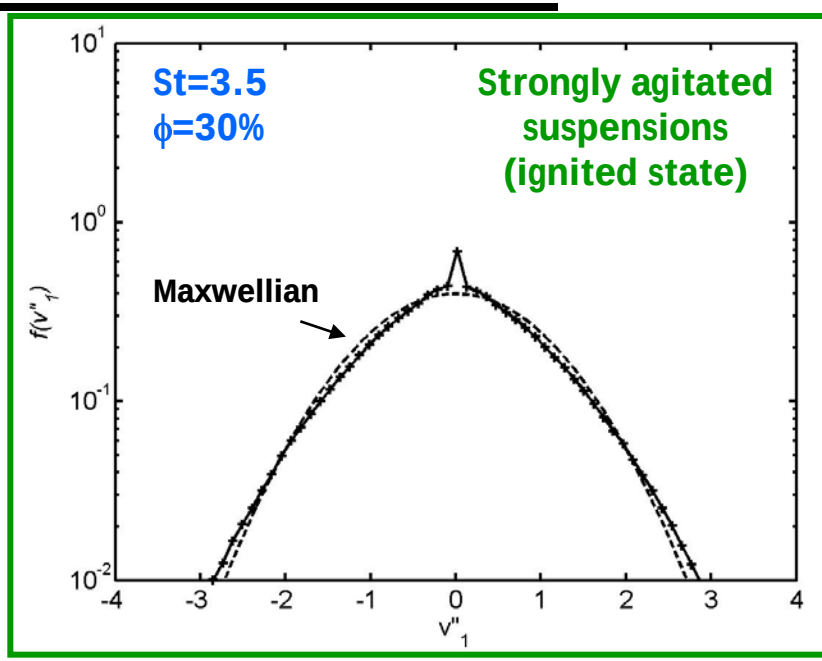
f(c,x) deviated Maxwellian ???

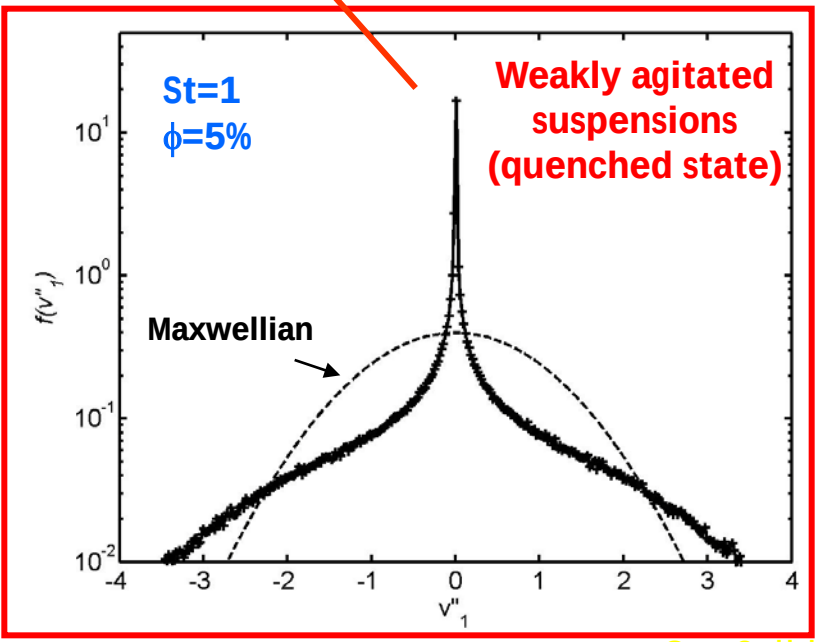
Theoretical solution

△✳□○ Simulation results

Kinetic theory of dense particulate flows







Gas-Solid

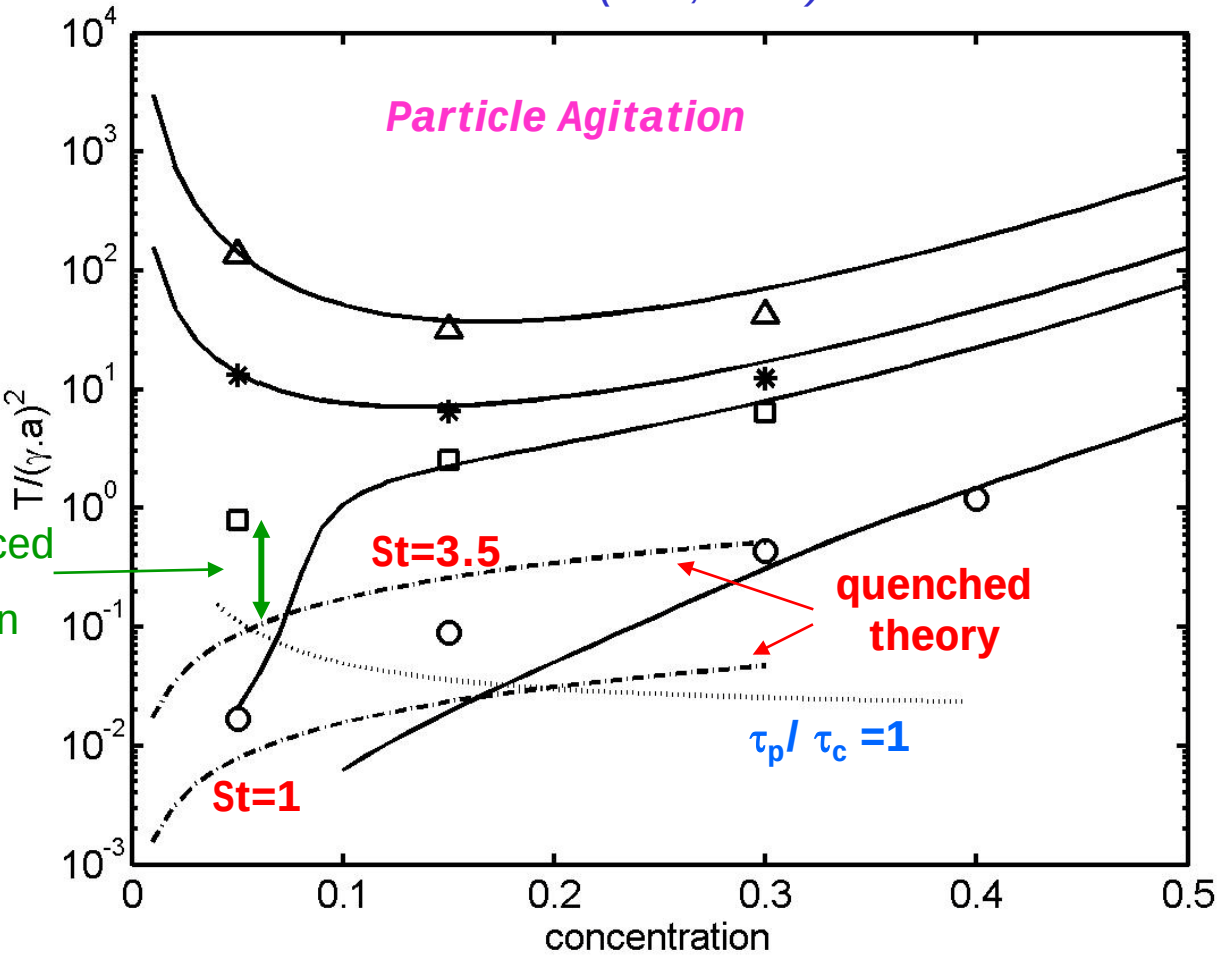
Different presumed pdf

Kinetic theory of dense particulate flows

(small St and ϕ) $\Leftrightarrow$ quenched theory

Same approach: substitute deviated Maxwellian with Dirac delta function

Tsao & Koch (JFM, 1995)



Difference reduced

Variance-driven collisions not considered

Kinetic theory of dense particulate flows

Eulerian prediction of the self-diffusion tensor in a shear flow:

$$D = \frac{1}{\varphi_a^{\,2} - \varphi_b \varphi_c} \begin{bmatrix} \varphi_a & -\varphi_c & 0 \\ -\varphi_b & \varphi_a & 0 \\ 0 & 0 & (\varphi_a^{\,2} - \varphi_b \varphi_c)/\varphi_a \end{bmatrix} \begin{bmatrix} T_{11} & T_{12} & 0 \\ T_{12} & T_{22} & 0 \\ 0 & 0 & T_{33} \end{bmatrix}$$

Kinetic stress tensor

$$\varphi_a = \frac{1}{\tau_p} + \frac{2}{3}\frac{(1+e)}{2}\frac{1}{\tau_c}$$

$$\varphi_b = -\left(\frac{8}{5}\phi g_0 \frac{(1+e)}{2}\right)\gamma$$

$$\varphi_c = \left(1 - \frac{8}{5}\phi g_0 \frac{(1+e)}{2}\right)\gamma$$

γ=0

$$D = \left(\frac{1}{\tau_p} + \frac{(1+e)}{3}\frac{1}{\tau_c}\right)^{-1} T$$

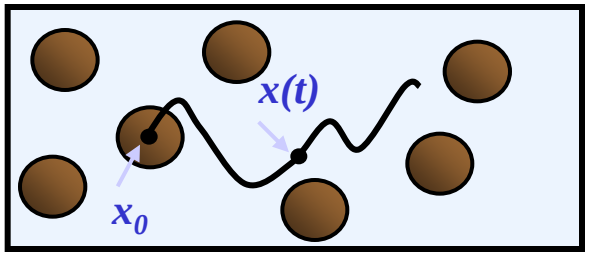
← *Laviéville, Deutsch and Simonin (1995)*

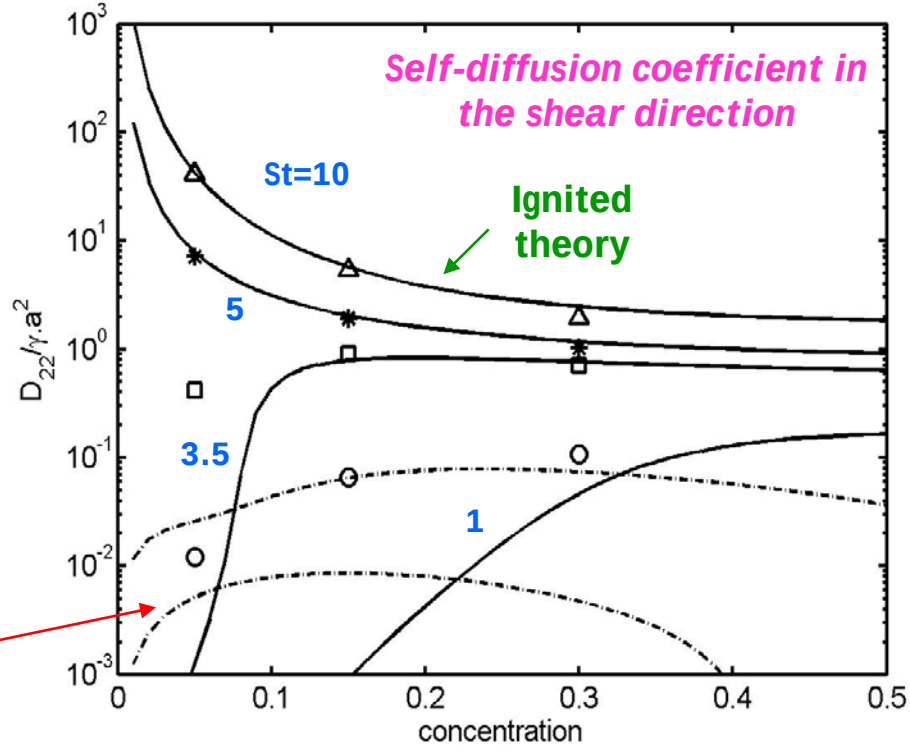
St→∞

$$D = \frac{3}{(1+e)}\tau_c T$$

← *Granular isotropic flow*

$$D_{ij} = \frac{1}{2}\lim_{t\to\infty}\frac{d}{dt}\left\langle \left(x_i(t) - x_j(0)\right)^2 \right\rangle$$



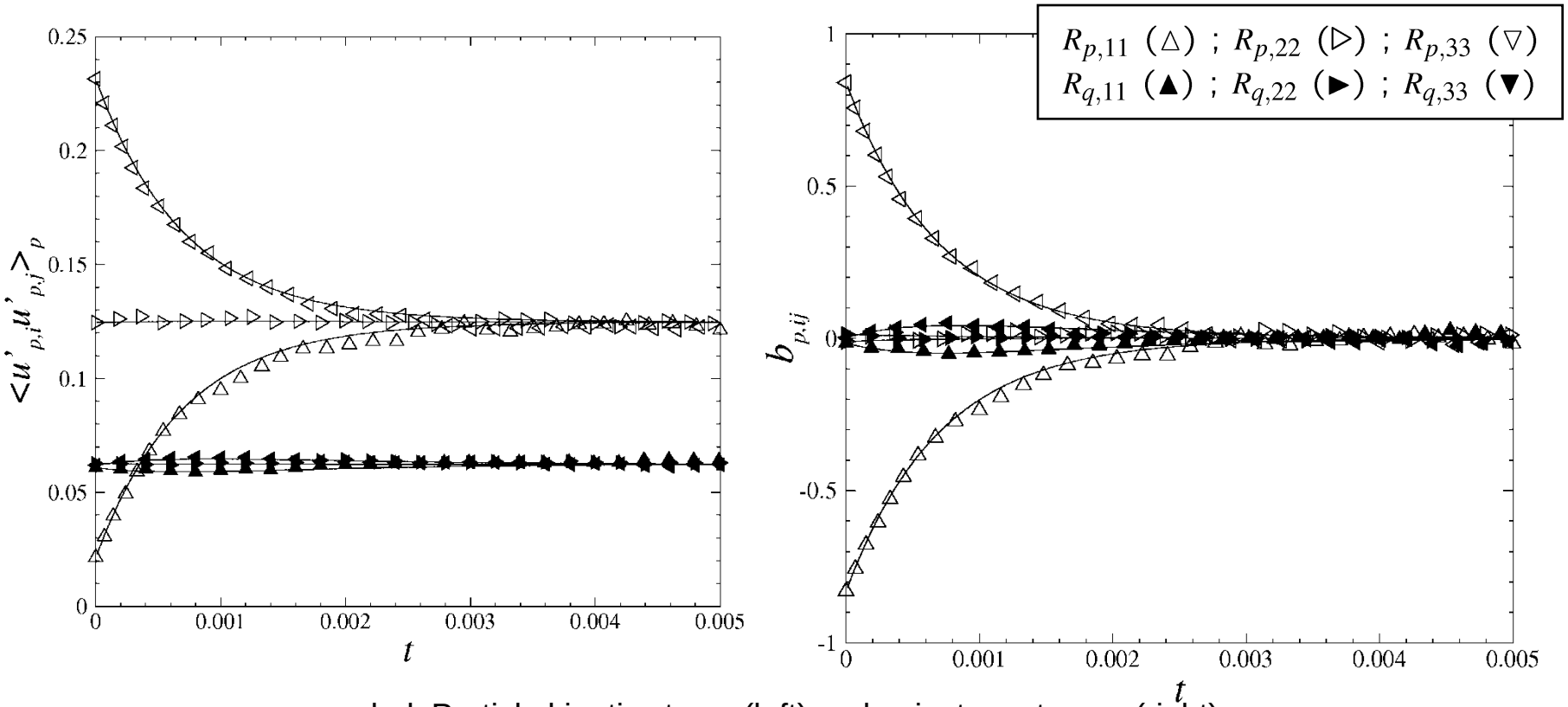


Kinetic theory of dense particulate flows

p-particle non-isotropic + *q*-particle isotropic

$$\beta_1 = 0.4 \;\; ; \quad \beta_2 = 1 \;\; ; \quad \beta_3 = \sqrt{3 - \beta_1^2 + \beta_2^2}$$
$$\gamma_1 = 1 \;\; ; \quad \gamma_2 = 1 \;\; ; \quad \gamma_3 = 1$$

$$\Rightarrow \quad m_p q_p^2 = m_q q_q^2$$



symbol: Particle kinetic stress (left) and anisotropy tensor (right)

——— : model predictions

Dry granular simulation and modeling of the redistribution effect between particle kinetic stresses in bidisperse solid mixture

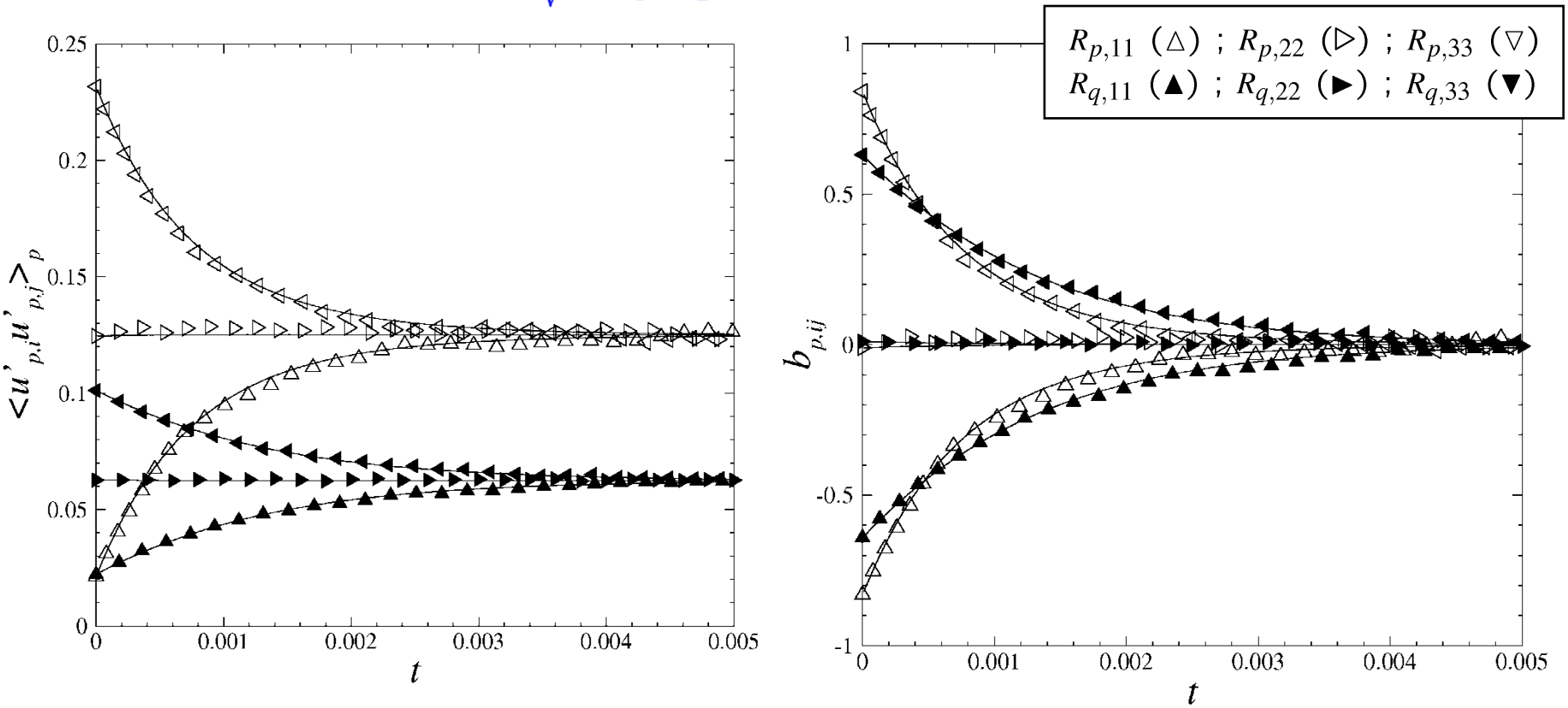
Kinetic theory of dense particulate flows

p-particle anisotropic + *q*-particle anisotropic

$$\beta_1 = 0.4 \;\; ; \;\; \beta_2 = 1 \;\; ; \;\; \beta_3 = \sqrt{3-\beta_1^2-\beta_2^2} \approx 1.35$$

$$\gamma_1 = 0.6 \;\; ; \;\; \gamma_2 = 1 \;\; ; \;\; \gamma_3 = \sqrt{3-\gamma_1^2+\gamma_2^2} \approx 1.28$$

$$\Rightarrow \; m_p q_p^2 = m_q q_q^2$$



symbol: Particle kinetic stress (left) and anisotropy tensor (right)

——— : model predictions

Dry granular simulation and modeling of the redistribution effect between particle kinetic stresses in bidisperse solid mixture

Outlines

- Direct numerical simulation of fluid-particle interactions
    + Flow simulation in fixed array of solid particles
    + VOF type simulation of a liquid-solid-fluidized bed

- Kinetic theory of particulate flows
    + Self-diffusion of particles with finite inertia
    + Polydisperse moment approach

- n-Eulerian modeling appraoch
    + « Coarse-grid » model development
    + Experimental validation and industrial application

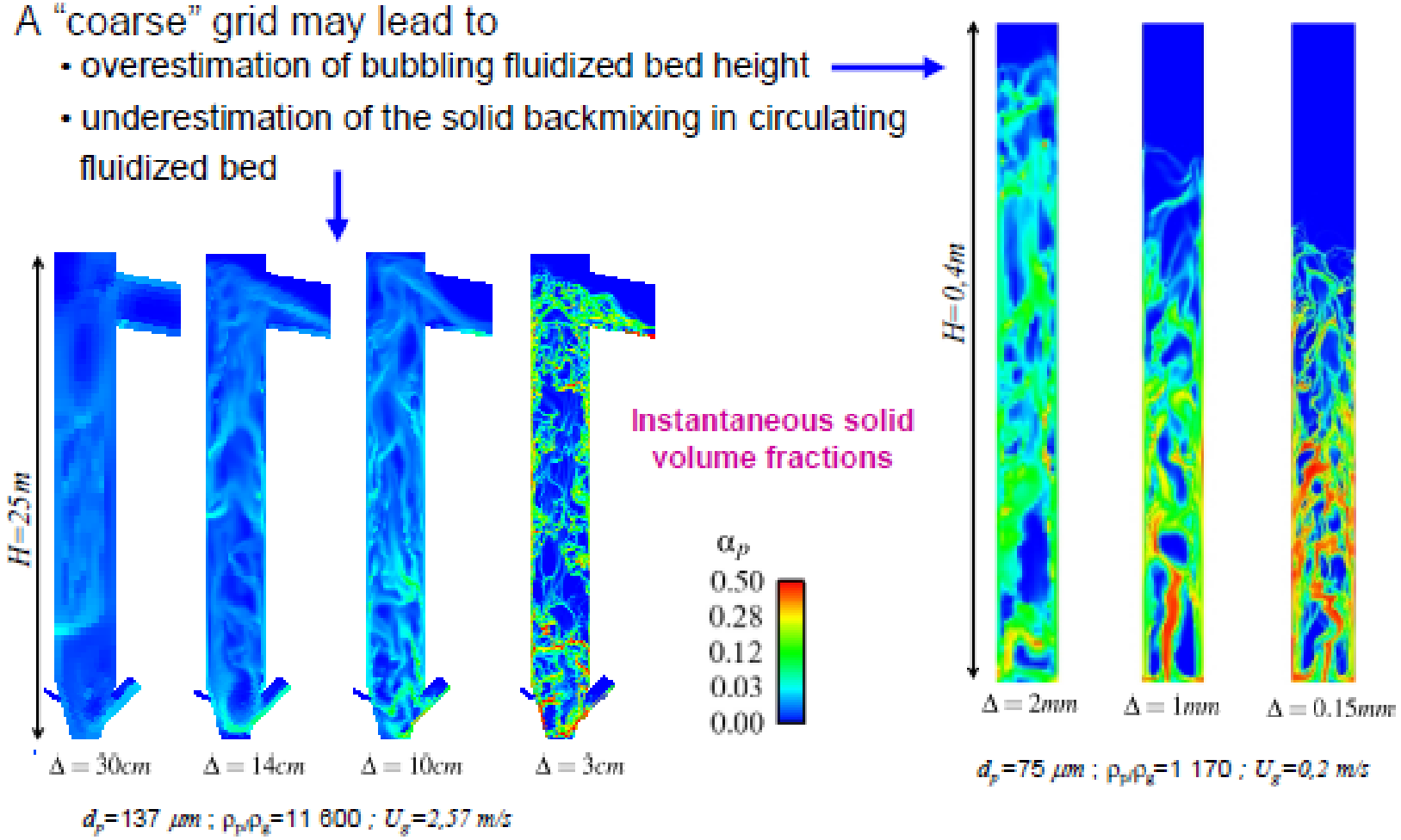
- Conclusion

Coarse-grid model development

Influence of the mesh refinement

A "coarse" grid may lead to

- overestimation of bubbling fluidized bed height
- underestimation of the solid backmixing in circulating fluidized bed



Development of subgrid model to account for the unresolved flow structure effects

Coarse-grid model development

Numerical Model

Multi-fluid model, implemented in NEPTUNE_CFD V1.07@TIse (*), written in the frame of kinetic approach of particulate flows with special developments to account for the effect of the interstitial gas.

- Mass balance equation (k=g: gas and k=p: particle)

$$\frac{\partial}{\partial t}(\alpha_k \rho_k) + \frac{\partial}{\partial x_j}(\alpha_k \rho_k U_{k,j}) = 0$$

- Momentum balance equation

Interfacial momentum transfer

Effective stress tensor

$$\frac{\partial}{\partial t}(\alpha_k \rho_k U_{k,i}) + \frac{\partial}{\partial x_j}(\alpha_k \rho_k U_{k,i} U_{k,j}) = -\alpha_k \frac{\partial P_g}{\partial x_i} + I_{k,i} + \alpha_k \rho_k g_i + \frac{\partial}{\partial x_j}\Sigma_{k,ij}$$

  - Interfacial momentum transfer

Fluid-particle drag force: $I_{p,i} = -I_{g,i} = -\alpha_p \rho_p \frac{U_{p,i} - U_{g,i}}{\tau_{gp}^F}$

with $\frac{1}{\tau_{gp}^F} = \frac{3}{4}\frac{\rho_g \langle C_D \rangle}{\rho_p \, d_p}\langle |\mathbf{V}_r| \rangle$ and $\langle C_D \rangle = \begin{cases} min\left[\left\langle C_D^{Wen\ \&\ Yu}\right\rangle, \left\langle C_D^{Ergun}\right\rangle\right] & \text{if } \alpha_p > 0.3 \\ \left\langle C_D^{Wen\ \&\ Yu}\right\rangle & \text{otherwise} \end{cases}$

  - Effective stress tensor
    - ✓ LES model for the gas
    - ✓ Two-equations model for the particles (q_p^2-q_{gp})

(*)The NEPTUNE_CFD code – with specific adaptations by IMFT - has been used to obtain the results presented here. NEPTUNE_CFD is developed in the framework of the NEPTUNE project, financially supported by CEA, EDF, IRSN and AREVA-NP.

Coarse-grid model development

Two-Fluid "LES" approach

1. **Decomposition** into resolved $\overline{X}$ and X'unresolved field

- Solid fraction: $\alpha_p = \overline{\alpha}_p + \alpha_p'$
- Filtered mean particle velocity: $\widetilde{U}_{p,i} = \dfrac{\overline{\alpha_p U_{p,i}}}{\overline{\alpha}_p}$
- Filtered mean gas velocity: $\widetilde{U}_{g,i} = \dfrac{\overline{\alpha_g U_{g,i}}}{\overline{\alpha}_g}$
- Filtered mean gas velocity seen by particles: $\widetilde{U}_{g@p,i} = \dfrac{\overline{\alpha_p U_{g,i}}}{\overline{\alpha}_p}$

2. Filtered drag term

$$\frac{\overline{\alpha_p \rho_p \left(U_{p,i} - U_{g,i}\right)}}{\tau_{gp}^F} \approx \frac{\overline{\alpha}_p \rho_p}{\overline{\tau}_{gp}^F} \left(\widetilde{U}_{p,i} - \widetilde{U}_{g,i} + \widetilde{V}_{d,i}\right)$$

Subgrid velocity: $\widetilde{V}_{d,i} = \widetilde{U}_{g,i} - \widetilde{U}_{g@p,i}$

Coarse-grid model development

3. Subgrid drift velocity model

General form: $$\widetilde{V}_{d,i} = g_{ij}(\overline{\alpha}_p, \widetilde{Re}_p, \Delta/\Delta_c) \times \left(\widetilde{U}_{p,j} - \widetilde{U}_{g,j}\right)$$

with $\widetilde{Re}_p = \dfrac{\overline{\alpha}_g d_p |\widetilde{V}_r|}{\mu_g}$, Δ the cell width and Δ_c a characteristic length scale.

- model #1: $$\widetilde{V}_{d,i} = g(\overline{\alpha}_p \widetilde{Re}_p, \Delta/\Delta_c) \times \left(\widetilde{U}_{p,i} - \widetilde{U}_{g,i}\right)$$

- model #2: $$\overline{\alpha}_p \widetilde{V}_{d,i} = K_{ij} \underbrace{f(\Delta/\Delta_c) h(\overline{\alpha}_p)}_{\text{From a priori analysis}} \times \left(\widetilde{U}_{p,j} - \widetilde{U}_{g,j}\right)$$

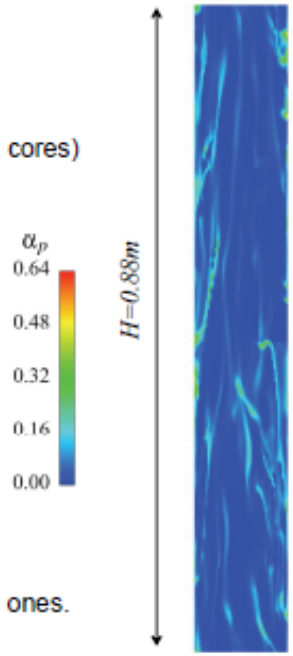
Dynamic model
(Germano et al., 1991)

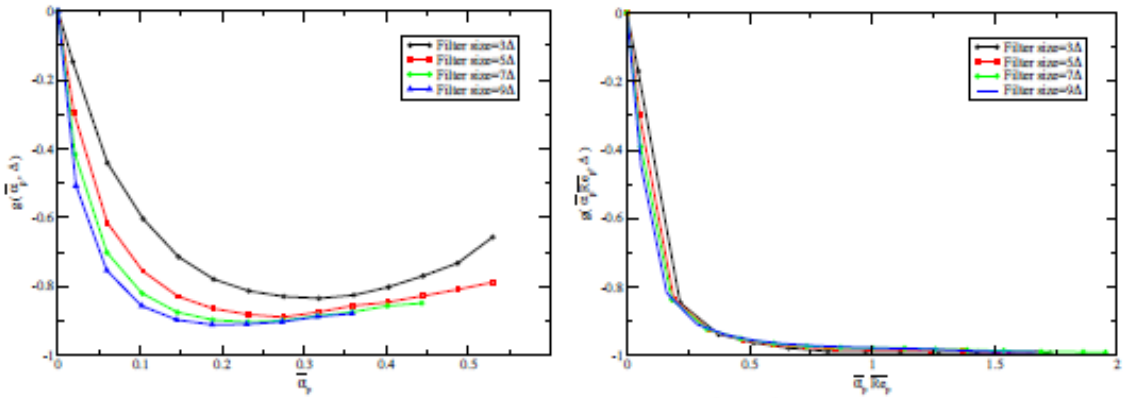
Coarse-grid model development

A priori Test: Fully resolved circulating fluidized bed

Numerical simulation parameters:

- 128×128×1024 cells (NEPTUNE_CFD parallel computation on 512 cores)
- Boundary conditions
  - Top and bottom: periodical
  - Otherwise: walls (pure slip)
- Imposed mean gas pressure gradient
- Gas properties
  - Density: ρ_g= 1.2 kg/m^3
  - Viscosity: μ_g= 1.82×10^{-5} $kg/m/s$
- Particle properties
  - Diameter: d_p= 70 μm
  - Density: ρ_p=1400 kg/m^3
  - Particle-particle collision restitution coefficient: e_c=0.9
  - Mean solid volume fraction α_p=0.05
- Filter applied to separate the unresolved quantities from the resolved ones.





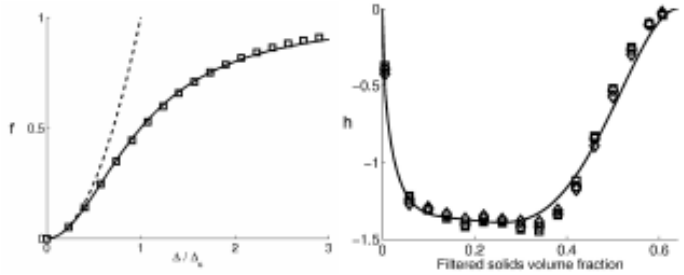
A priori analysis of subgrid drag contribution model #1

Coarse-grid model development

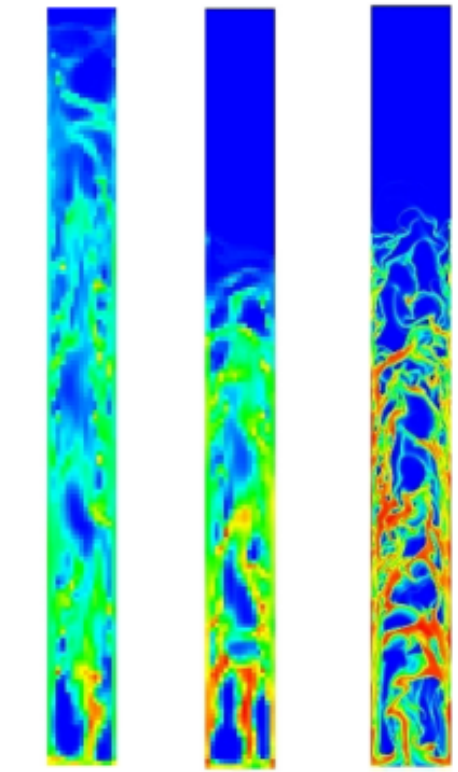
A posteriori Test: CFD prediction of bubbling fluidized bed

Numerical simulation parameters:

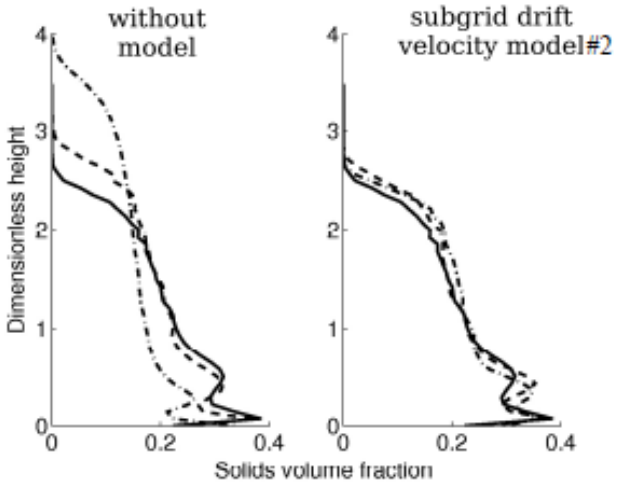
- Gas properties
  - Density: $\rho_g = 1.2\ kg/m^3$
  - Viscosity: $\mu_g = 1.82 \times 10^{-5}\ kg/m/s$
  - Fluidization velocity: $U_g = 0,2\ m/s$
- Geldart A particles
  - Diameter: $d_p = 75\ \mu m$
  - Density: $\rho_p = 1500\ kg/m^3$
- Subgrid drag contribution model#2



Given functions f (left) and h (right) used for the subgrid drift velocity model#2



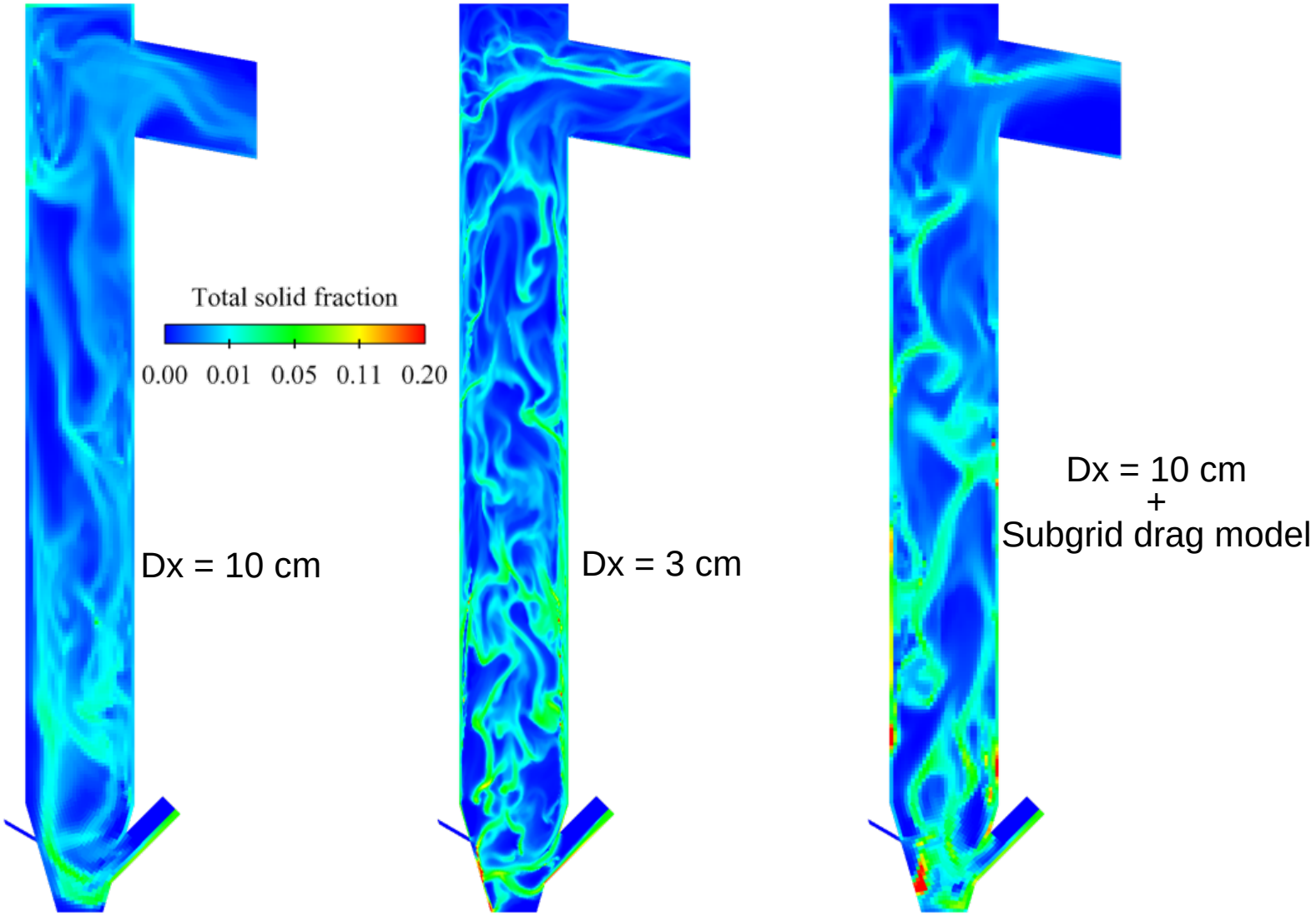
Without model | With model#2 | Fully resolved



Vertical profiles of the time-averaged solid volume fraction without (left) and with (right) subgrid drift velocity model: influence of the mesh refinement, (——) fully resolved simulation results

Coarse-grid model development

A posteriori test: CFD prediction of a circulating fluidized bed



Experimental validation

3D simulation of pressurized fluidized bed

Comparison with experimental data obtained by PEPT

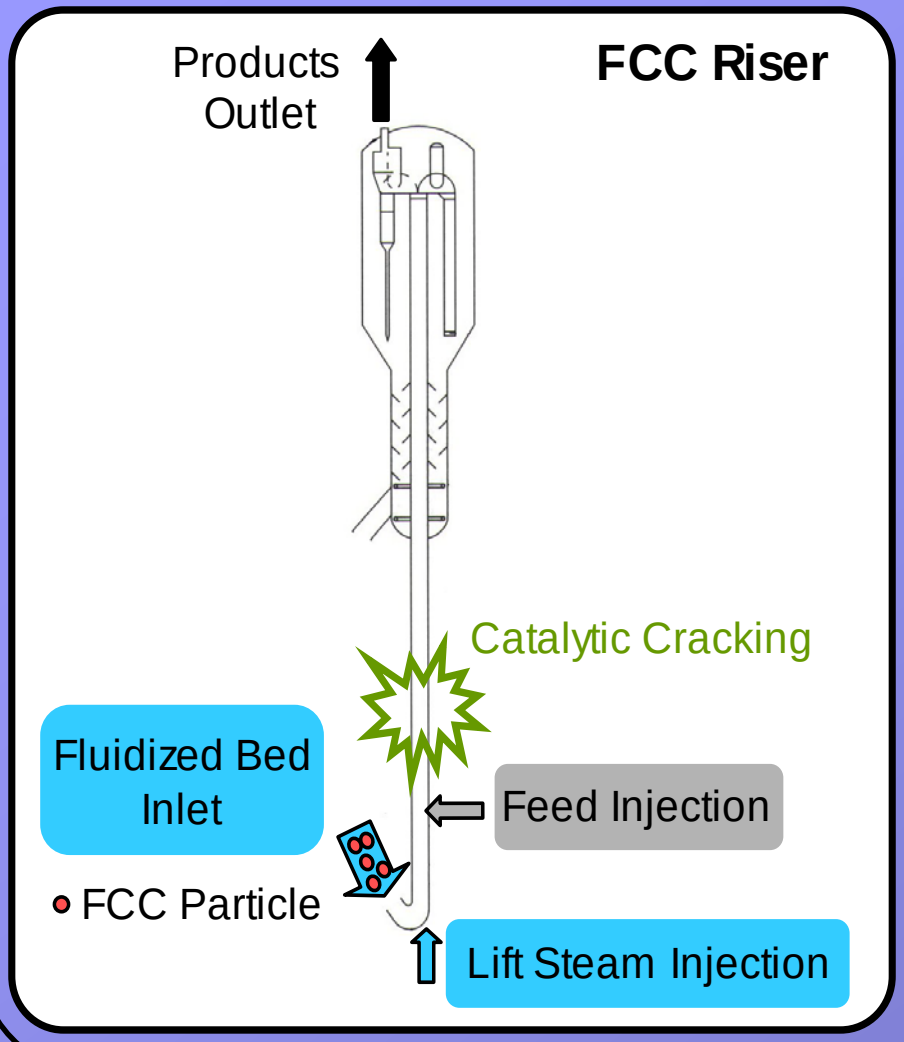
[1]P. Fede, [1]G. Moula, [2]A. Ingram, [3]T. Dumas, [1]O. Simonin

1: Institut de Mécanique des Fluides de Toulouse - Écoulements Et Combustion
CNRS UMR5502-INPT/ENSEEIHT-UPS Toulouse, France

2: Chemical Engineering, The University of Birmingham
Birmingham B15 2TT, U.K

3: 4INEOS; Innov`ene; CTL/PRO Ecopolis Lavéra, F-13117, Lavéra, France

MULTIPHASE FLOW SIMULATION OF FCC RISER



FEED INJECTION ZONE

INTEREST

- Crucial Zone for All Processes

PROPERTIES

- Three phases :
  - Gas : Steam, Feed Vapor
  - Liquid : Feed Droplets
  - Solid : FCC Particles
- Heat and Mass Transfer :
  - "Hot" Bed / "Cold" Feed
  - Feed Droplet Evaporation
  - Chemical reaction

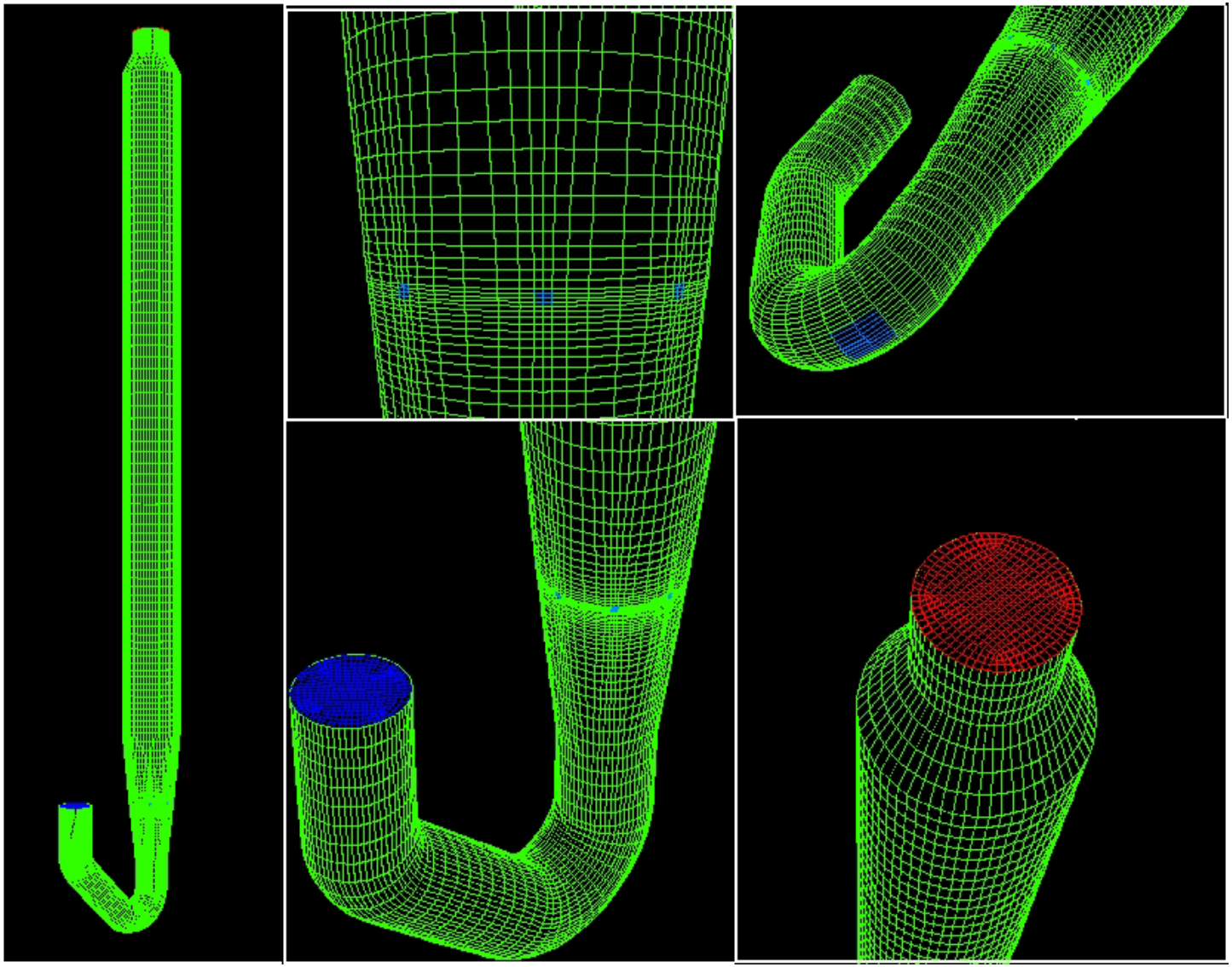
GOAL

- Increasing Three-Phase Heat and Mass Transfer Comprehension

IMFT INSTITUT DE MECANIQUE DES FLUIDES DE TOULOUSE

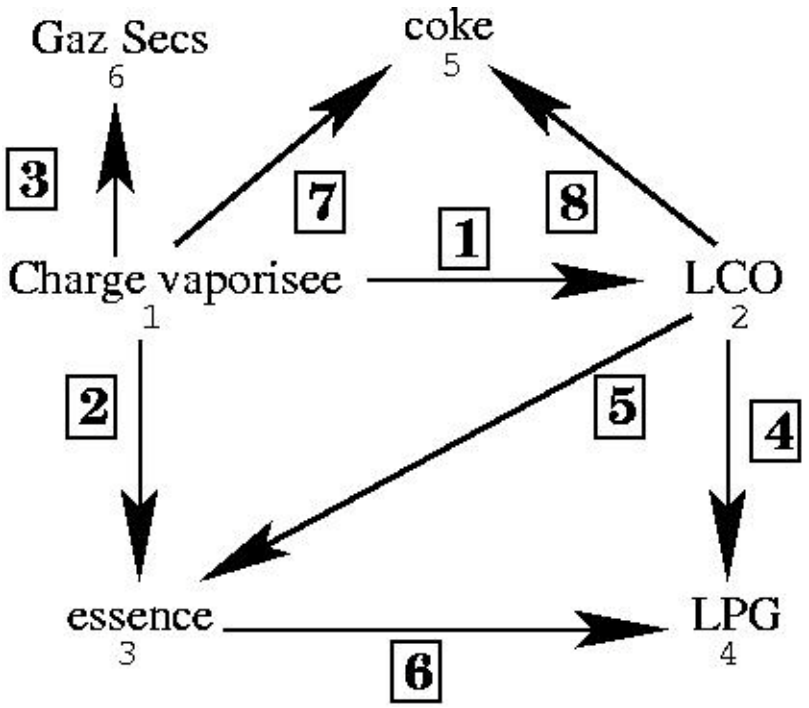
TOTAL

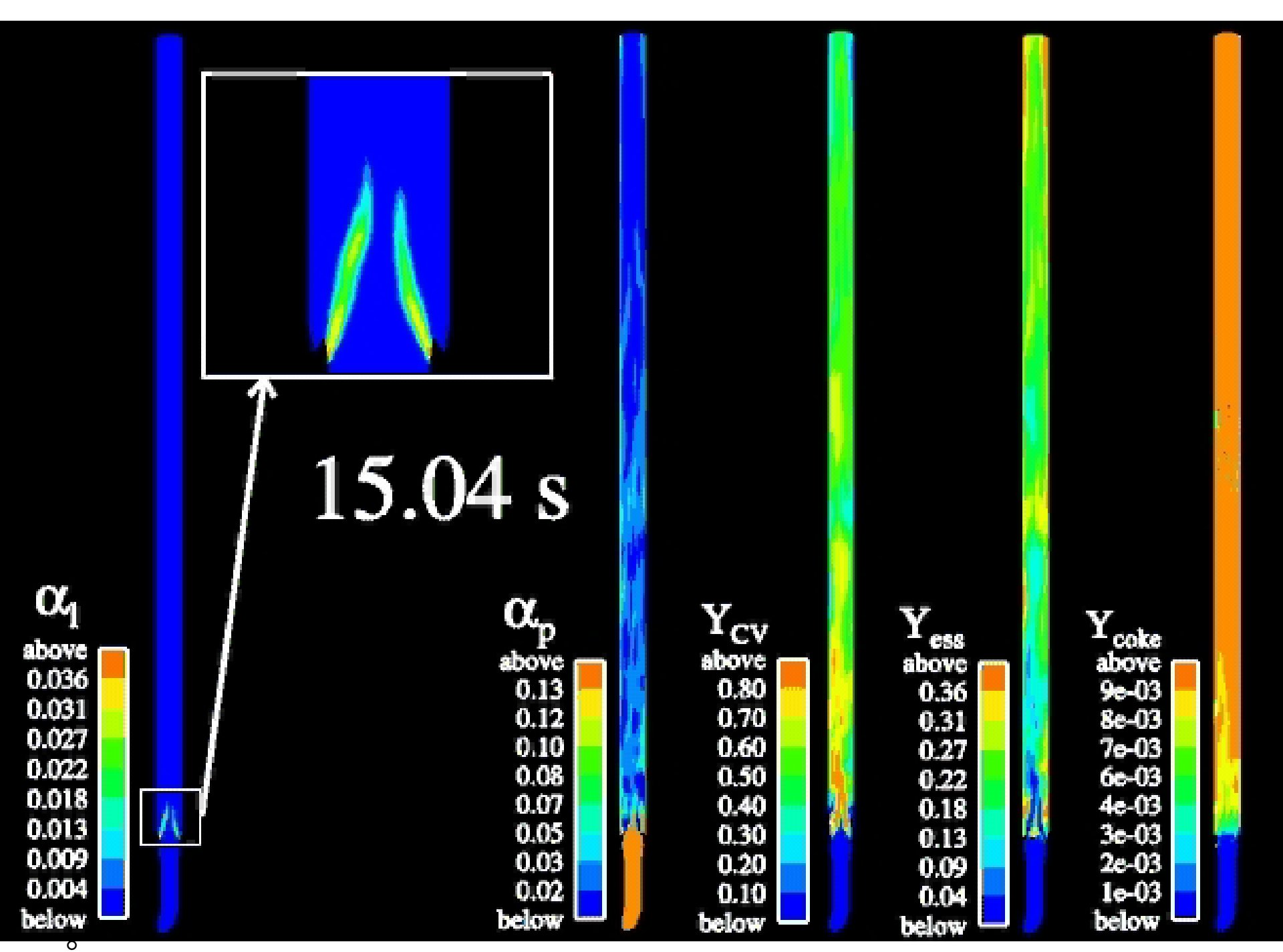
3D Unsteady Reactive Simulation



3D Unsteady Reactive Simulation of Feed Injection in FCC

den Hollander modified model




15.04 s
α_l
above
0.036
0.031
0.027
0.022
0.018
0.013
0.009
0.004
below
α_p
above
0.13
0.12
0.10
0.08
0.07
0.05
0.03
0.02
below
Y_{CV}
above
0.80
0.70
0.60
0.50
0.40
0.30
0.20
0.10
below
Y_{ess}
above
0.36
0.31
0.27
0.22
0.18
0.13
0.09
0.04
below
Y_{coke}
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6e-03
4e-03
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2e-03
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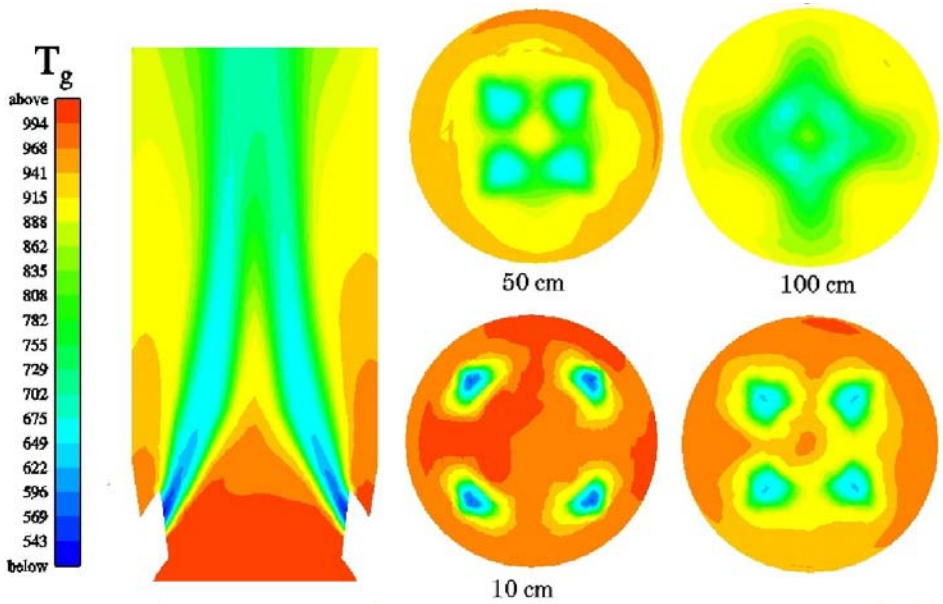
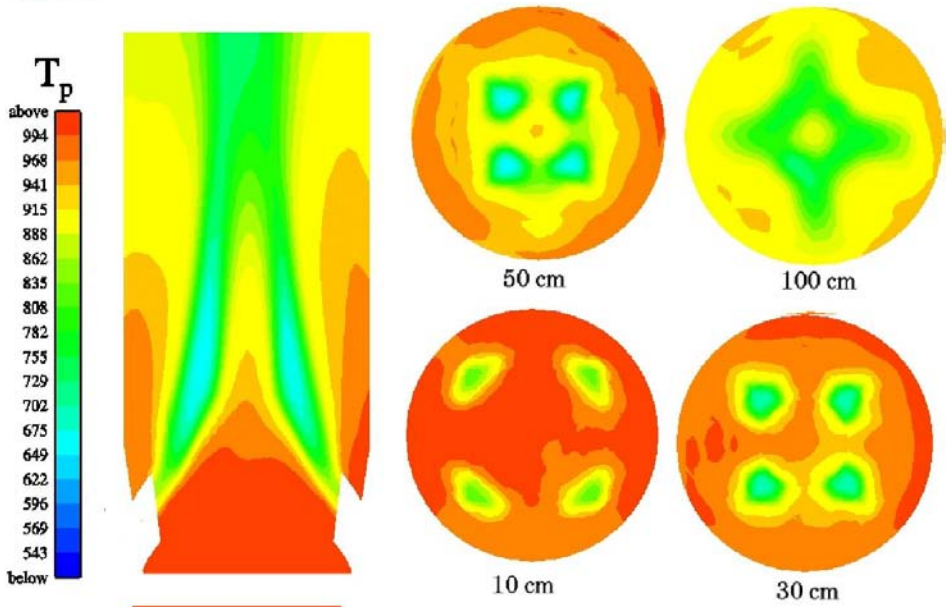
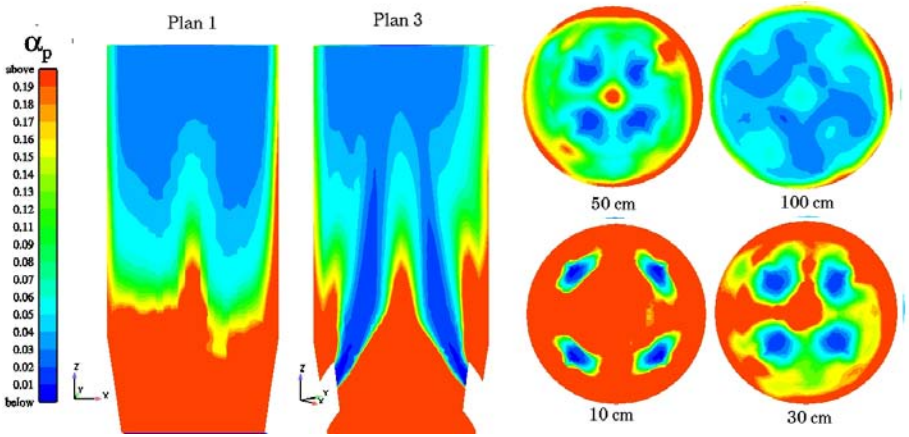


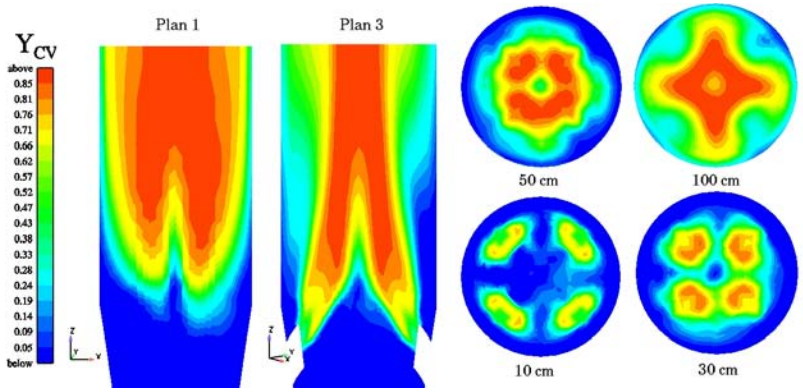
Time-averaged temperature of the gaseous mixture

Time-averaged temperature of the catalyst particles

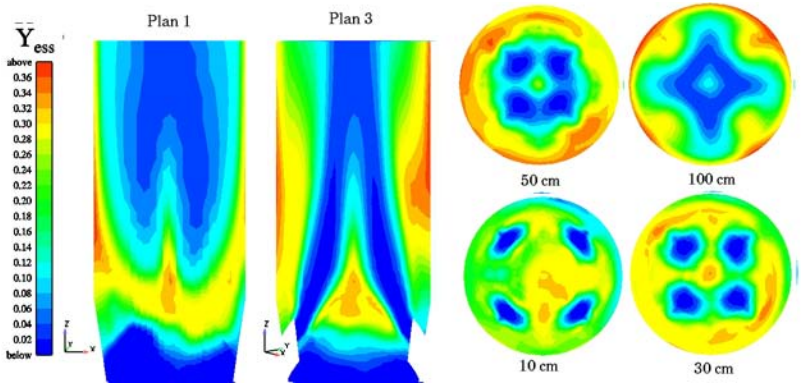




Time-averaged volumetric fraction of catalyst particles



Time-averaged massic fraction of vaporized feed



Time-averaged massic fraction of gazoline

Multiphase model development perspectives

Microscopic drag and heat transfer coefficients in polydispersed mixture

Reactive multi-phase flows (coupling with chemical reactions)

Statistical particle-particle interaction model (frictional or smooth particles)

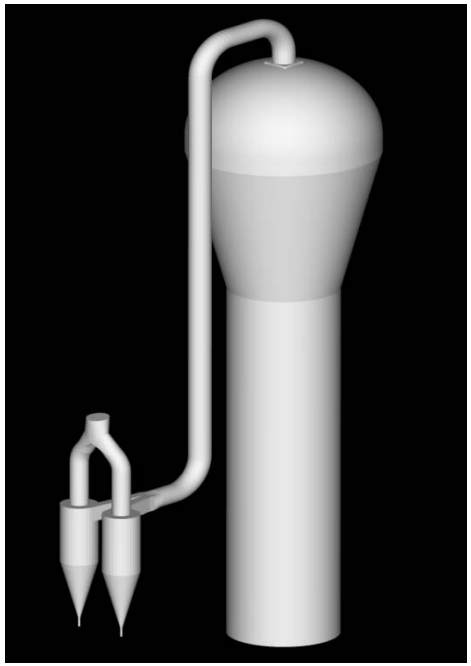
Smooth and rough wall boundary conditions (mass, momentum and heat transfer)

Subgrid models for reactive polydispersed particulate flows

Simulation de l'écoulement dans « cyclones + tuyauterie »

- **Simulation réalisée sur le supercalculateur Hyperion de CALMIP (Nehalem) sur 16 cœurs (Xeon X5560 2,8 GHz)**
- **Maillage de 149 364 cellules**
- **Vitesse d'entrée rapide (~15 $m.s^{-1}$) => vitesse maximum ~40 $m.s^{-1}$**
- **Cellules relativement petites (de 5 cm à 5 mm)**
- **Nombre de Courant : $CFL=U*\Delta t/\Delta x=1 \Rightarrow \Delta t= \Delta x/U \sim 5.10^{-4}$ s**
- **1 seconde de temps physique ⇔ 1 500 itérations ⇔ 11 h CPU**
- **450 secondes de temps physique ⇔ 206 j CPU sur 1 cœur**
  ⇔ 13 j CPU en parallèle sur 16 coeurs

Simulation de l’écoulement sur la géométrie complète



- **Décomposition de la géométrie complète en sous éléments :**
  - **Réacteur Innovène 4**
  - **Tuyauterie**
  - **2 cyclones avec une sortie commune unique**

- **Maillage du Innovène 4**
  - Maillage de type Ogrid 2ème génération :
    ~ 1 300 000 cellules hexaèdriques - $\Delta x \sim \Delta y \sim$ 6 cm $\Delta z \sim$ 8 cm

-**Maillage de la tuyauterie**
  - Maillage de type Ogrid
    ~ 150 000 cellules hexaèdriques - $\Delta x \sim \Delta y \sim \Delta z \sim$ 5 cm

- **Maillage des cyclones**
  - Maillage de type Ogrid
    ~ 150 000 cellules hexaèdriques - $\Delta x \sim \Delta y \sim$ 5 à 0,5 cm $\Delta z \sim$ 8 cm

Simulation de l'écoulement sur la géométrie complète

Simulation réalisée :
- sur le superculateur JADE du centre de calcul national du CINES sur 256 cœurs (JADE : SGI Altix ICE de 12 288 cœurs Core2Quad E5472)
- sur le supercalculateur Hyperion de CALMIP (Nehalem) sur 256 cœurs (Xeon X5560 2,8 GHz)

~ 1 600 000 cellules

Vitesse maximum élevée ~ 40 $m.s^{-1}$

Cellules relativement petites (de 5 cm à 5 mm)

Nombre de Courant : $CFL=U*\Delta t/\Delta x=1 \Rightarrow \Delta t= \Delta x/U \sim 5.10^{-4}$ s

1 seconde de temps physique ⇔ 1 300 itérations ⇔ 15 j CPU sur 1 coeurs
⇔ 3 h en parallèle sur 256 coeurs

120 secondes de temps physique ⇔ 1800 j CPU en séquentiel (~5 ans)
⇔ 360h CPU en parallèle sur 256 cœurs (15j CPU)