Modelling of test case particle-laden jet with NEPTUNE_CFD

H. D. Le[1,2], J-M. Lacome[1], A. Vignes[1], B. Debray[1], B. Truchot[1],
P. Fede[2,3] , E. Climent[2,3]

[1]INERIS, Parc technologique ALATA, B.P. 2, FR-60550 Verneuil-en-Halatte
[2]Université de Toulouse ; INPT , UPS; IMFT, Allée du Professeur Camille Soula, 31400 Toulouse
[3]CNRS ; UMR5502 IMFT ; FR-31400 Toulouse, France

Email: hongduc.le@imft.fr

14th Workshop on Two-Phase Flow Predictions
September 7th -10th 2015

cnrs dépasser les frontières

IMFT INSTITUT DE MECANIQUE DES FLUIDES DE TOULOUSE

Université Fédérale Toulouse Midi-Pyrénées

INERIS maîtriser le risque pour un développement durable

Outline

I. Introduction
   1. Thesis context
   2. Test case

II. Theoretical model used by NEPTUNE_CFD
   1. Governing equations
   2. Closure models

III. Numerical simulation by NEPTUNE_CFD
   1. Geometry
   2. Mesh and boundary conditions
   3. Numerical results

IV. Conclusions

I. Introduction

Thesis context

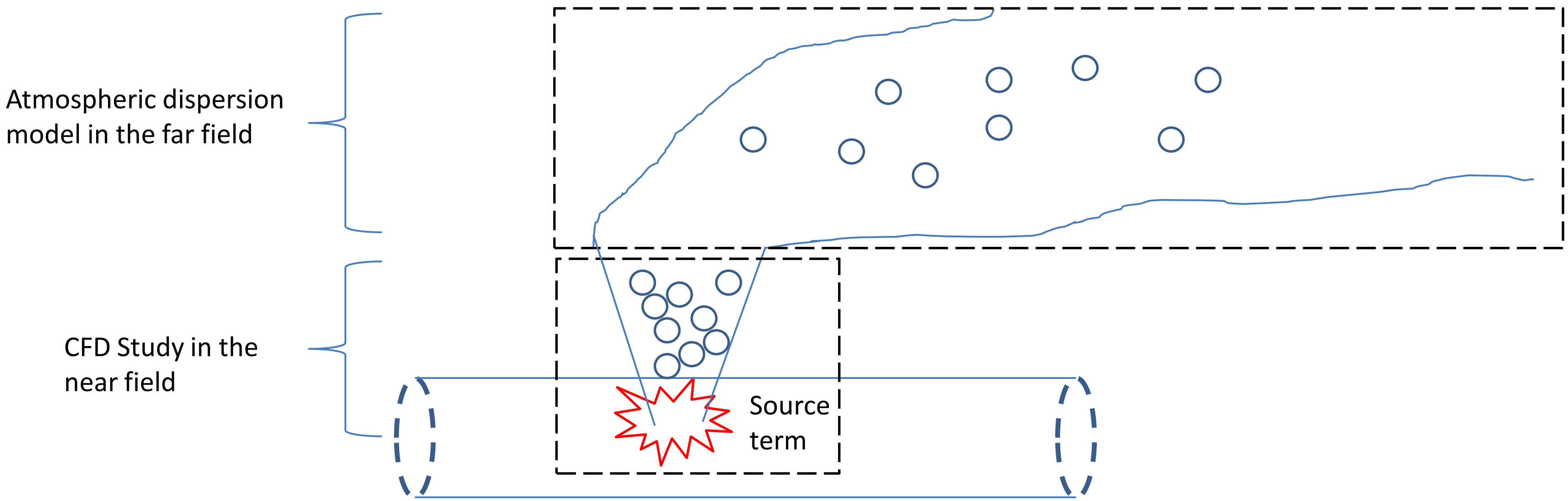
Thesis subject: Modelling of pressurized jet loaded with nanoparticles.

- Rapidly increase of use of nanotechnology in industrial process
- Application in safety management

Collaboration between:

- **INERIS** : Institut National de l’Environnement Industriel et des Risques
- **IMFT** : Institut de Mécanique des Fluides de Toulouse

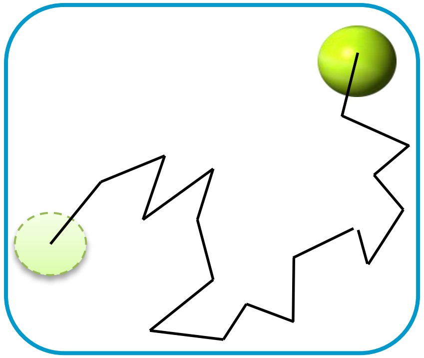
Accidental configuration: leakage of conveying pipe of nanoparticle



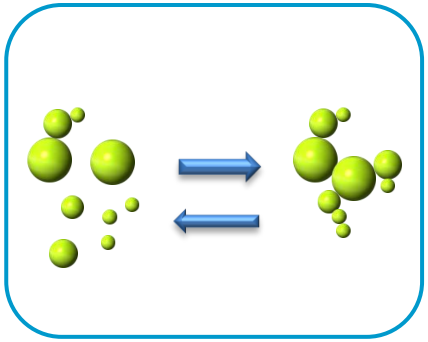
Thesis started day : January 05th 2015

Thesis context

Phenomena involved in nanoparticle dispersion:



Brownian motion



Agglomeration - Deagglomeration

Additional physical modelling of particulate jet:

- Drag
- Influence of particles on fluid turbulence
- Collision between particles
- Gravity, etc…

Numerical simulation tools currently used:

➢**NEPTUNE_CFD V2.0** supported by CEA (Commissariat à l'Energie Atomique), EDF (Electricité de France), IRSN (Institut de Radioprotection et de Sûreté Nucléaire) and AREVA which use Euler multifluid approach – RANS.

➢**Code_Saturne v4.0** developped by EDF which uses Euler – Lagrange approach – RANS/LES.

Thesis approach:

➢Numerical simulation of **microparticle** dispersion before numerical simulation of **nanoparticle** dispersion

➢Implementation of modelling of Brownian motion and agglomeration in numerical simulation tools

Test case

Aim of the test case: Evaluation of numerical simulation tool NEPTUNE_CFD V2.0.

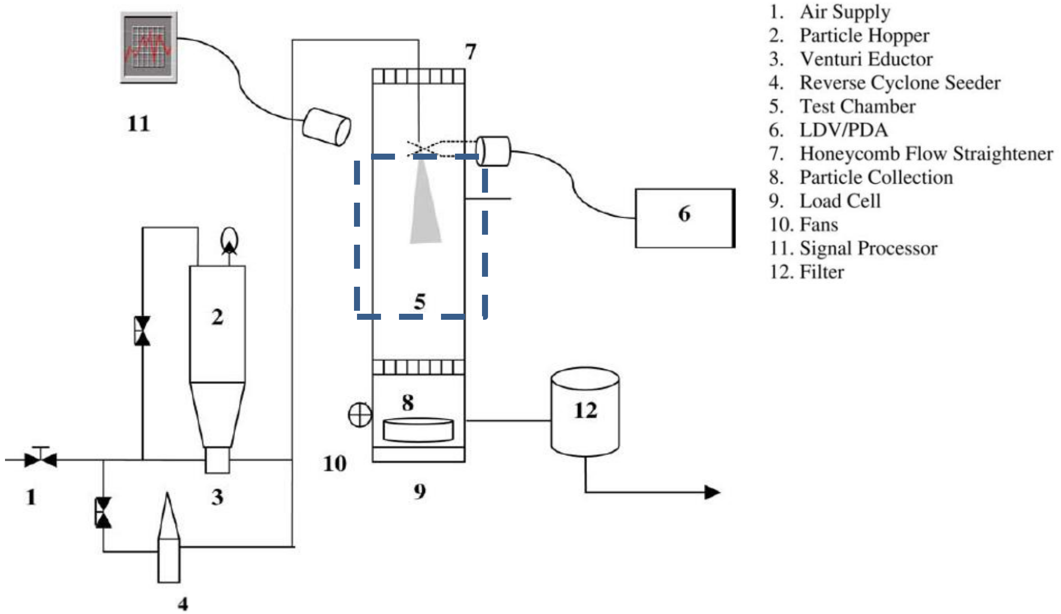
4 flow configurations:

- Single phase flow of gas
- Two-phase flow with 25 µm particles
- Two-phase flow with 70 µm particles
- Two-phase flow with binary mixture (25 µm particles and 70 µm particles)

Available experimental data provived by the Workshop Committee:

- Velocity of gas and particulate phases at nozzle exit and at centre line
- Velocity of particulate phase at axial positions of X/D=5, 10 and 15

D: nozzle diameter



Experimental setup from Hadinoto et al. 2005[1]

Numerical simulation domain

$$Re \approx 8{,}400$$

[1] Hadinoto, K., Jones, E. N., Yurteri, C., Curtis, J. S., 2005. INT J MULTIPHAS FLOW, 31: 416-424.

II. Theoretical models used by NEPTUNE_CFD

Governing equations

Unsteady eulerian multifluid approach for gas phase and particulate phase[1]:

➢**Continuous phase**: derived from local instant conservation equations in single-phase flow by density-weighted averaging (Favre averaging)

➢**Particulate phase**: derived in the frame of the kinetic theory of granular media based on a statistical approach using a Probality Density Function (PDF)

Balance equations are solved for each phase:

➢Mass balance

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

➢Momentum balance

$$\alpha_k \rho_k \left[\frac{\partial U_{k,i}}{\partial t} + U_{k,j} \frac{\partial U_{k,i}}{\partial x_j} \right] = \frac{\partial}{\partial x_j}\left[-\alpha_k \rho_k \left\langle u'_{k,i} u'_{k,j} \right\rangle \right] + \alpha_k \rho_k g_i + \alpha_k \frac{\partial P_g}{\partial x_i} + \sum_{k'=g,p} I_{k' \to k,i}$$

Need to be modelled!

$I_{k' \to k,i}$ Momentum exchange of gas-particles and particles-particles phases

$k = g : gas\ phase$

$k = p : particulate\ phase$

[1] Balzer, G.; Boëlle, A. & Simonin, O., 1995. Proc. Int. Sym. Engn. Foundation, 1125-1134

Closure models for momentum exchange

Momentum transfer between gas and particulate phase [1]

$$I_{g\rightarrow p,i} = -\frac{\alpha_p \rho_p}{\tau_{gp}^F} V_{r,i}$$

Drag model

Relaxation time of particles τ_{gp}^F

$$\frac{1}{\tau_{gp}^F} = \frac{3}{4}\frac{\rho_g}{\rho_p}\frac{\langle |v_r| \rangle}{d_p} C_d$$

Mean relative velocity of gas-particle

$$V_{r,i} = U_{p,i} - U_{g,i} - V_{d,i}$$

Wen and Yu model[2] for C_d

$$C_d = \begin{cases} \frac{24}{\mathrm{Re}_p}\left(1+0.15\,\mathrm{Re}_p^{0.687}\right)\alpha_g^{-1.7} & \mathrm{Re}_p < 1000 \\ 0.44\alpha_g^{-1.7} & \mathrm{Re}_p \geq 1000 \end{cases}$$

[1] Balzer, G., 2000. *Powder Technol*, *113*(3), 299-309.
[2]Wen, C.Y. and Yu, Y.H., 1966., Chem. Eng. Pog. Sym., 62, 110-111

Closure models for momentum exchange

Momentum transfer between particles [1]

$$I_{q\rightarrow p,i} = -\frac{m_p m_q}{m_p + m_q}\frac{1+e_c}{2}\frac{n_p}{\tau_{pq}^c}\left(U_{p,i} - U_{q,i}\right) H_1(z)$$

e_c Coefficient of restitution

$e_c = 0.9$ For the test case

Collision characteristic time

$$\frac{1}{\tau_{pq}^c} = \pi n_q d_{pq}^2 g_r$$

Model approximation

$$H_1(z) = \frac{8+3z}{6+3z}$$

Particle mean relative velocity at impaction

$$g_r = \sqrt{\frac{16}{\pi}\frac{2}{3}q_r + U_{pq,i}U_{pq,i}}$$

Model parameter

$$z = \frac{3U_{pq,i}U_{pq,i}}{8q_r}$$

Particle mean agitation

$$q_r = \frac{1}{2}\left(q_p^2 + q_q^2\right)$$

Particle mean relative velocity

$$U_{pq,i} = U_{p,i} - U_{q,i}$$

[1] Gourdel, C., Simonin, O., Brunier, E., 1999.. In 6 Int Conf. on circulating fluidized beds.
[2] Lun C. , Savage S. , 1986. Acta Mech. 63 1986. 15–44.

Closure models for turbulence

Fluid turbulence model[1] $k-\varepsilon$

*Turbulence created by wake of particulate phase is not considered.

$$\alpha_g\rho_g\left[\frac{\partial k}{\partial t}+U_{g,j}\frac{\partial k}{\partial x_j}\right]=\frac{\partial}{\partial x_j}\left[\alpha_g\rho_g\frac{\nu_g^t}{\sigma_k}\frac{\partial k}{\partial x_j}\right]-\alpha_g\rho_g\varepsilon-2k\frac{\partial U_{g,i}}{\partial x_j}+\sum_p\Pi_{p\to g}^k$$

$$\alpha_g\rho_g\left[\frac{\partial \varepsilon}{\partial t}+U_{g,j}\frac{\partial \varepsilon}{\partial x_j}\right]=\frac{\partial}{\partial x_j}\left[\alpha_g\rho_g\frac{\nu_g^t}{\sigma_\varepsilon}\frac{\partial \varepsilon}{\partial x_j}\right]-\alpha_g\rho_g\frac{\varepsilon}{k}\left[C_{\varepsilon,1}\left\langle u'_{g,i}u'_{g,j}\right\rangle\frac{\partial U_{g,i}}{\partial x_j}+C_{\varepsilon,2}\varepsilon\right]+\sum_p\Pi_{p\to g}^\varepsilon$$

Reynolds tensor of gas phase (Boussinesq approximation)

$$\left\langle u'_{g,i}u'_{g,j}\right\rangle=-\nu_g^t\left[\frac{\partial U_{g,i}}{\partial x_j}+\frac{\partial U_{g,j}}{\partial x_i}\right]+\frac{2}{3}\left[k+\nu_g^t\frac{\partial U_{g,m}}{\partial x_m}\right]\delta_{ij}$$

Model constants

$$C_{12}=0.34, C_\mu=0.09, \sigma_k=1, \sigma_\varepsilon=1.3$$
$$C_{\varepsilon1}=1.44, C_{\varepsilon2}=1.92, C_{\varepsilon3}=1.2$$

Influence of particles in fluid turbulence: two-way coupling

$$\Pi_{p\to g}^k=\frac{\alpha_p\rho_p}{\alpha_g\rho_g}\frac{1}{\tau_{gp}^F}\left[q_{gp}-2k+V_{d,i}V_{r,i}\right]\qquad \Pi_{p\to g}^\varepsilon=C_{\varepsilon,3}\frac{\varepsilon}{k}\Pi_{p\to g}^k$$

[1]Elghobashi, S. E., & Abou-Arab, T. W., 1983. *Physics of Fluids (1958-1988)*, *26*(4), 931-938.

Closure models for turbulence

Kinetic energy transport equation [1]

Diffusion of kinetic energy

Production by gradient of the mean of velocity

Interaction with gas phase

$$\alpha_p \rho_p \left[\frac{\partial q_p^2}{\partial t} + U_{p,j} \frac{\partial q_p^2}{\partial x_j} \right] = \frac{\partial}{\partial x_j} \left[\alpha_p \rho_p \left(K_p^{kin} + K_p^{col} \right) \frac{\partial q_p^2}{\partial x_j} \right] - \left\langle u'_{p,i} u'_{p,j} \right\rangle \frac{\partial U_{p,i}}{\partial x_j} - \frac{\alpha_p \rho_p}{\tau_{gp}^F} \left[2 q_p^2 - q_{gp} \right] + \sum_q \varepsilon_{qp} + \sum_q \chi_{qp}$$

Granular stress tensor [2]

Dissipation by inelastic collision

Agitation exchange between particles

$$\left\langle u'_{p,i} u'_{p,j} \right\rangle = -\mu_p \left[\frac{\partial U_{p,i}}{\partial x_j} + \frac{\partial U_{p,j}}{\partial x_i} - \frac{2}{3} \frac{\partial U_{p,m}}{\partial x_m} \delta_{ij} \right] + \left[P_p - \lambda_p \frac{\partial U_{p,m}}{\partial x_m} \right] \delta_{ij}$$

Granular viscosity

$$\mu_p = \alpha_p \rho_p \left(\nu_p^{kin} + \nu_p^{col} \right)$$

K_p^{kin}	Kinetic diffusivity	ν_p^{kin}	Granular kinetic viscosity	P_p	Granular pressure
K_p^{col}	Collisional diffusivity	ν_p^{col}	Granular collisonal viscosity	λ_p	Bulk viscosity

[1]Boëlle, A., Balzer, G., Simonin, O., 1995. ASME FED, Gas–Solid Flow 228. 9–18.
[2]Balzer, G., 2000. Powder Technology 113 299-309

Closure models for turbulence

Transport equation of correlation fluid particle velocity fluctuation[1]

Turbulent transport by fluctuation

Production by gradient of the mean velocity of gas and particulate phase

$$\alpha_p \rho_p \left[\frac{\partial q_{gp}}{\partial t} + U_{p,j} \frac{\partial q_{gp}}{\partial x_j} \right] = \frac{\partial}{\partial x_j} \left[\alpha_p \rho_p \frac{\nu^t_{gp}}{\sigma_{q_{gp}}} \frac{\partial q_{gp}}{\partial x_j} \right] - \alpha_p \rho_p \left\langle u'_{g,i} u'_{p,j} \right\rangle \frac{\partial U_{p,i}}{\partial x_j} - \alpha_p \rho_p \left\langle u'_{g,j} u'_{p,i} \right\rangle \frac{\partial U_{g,i}}{\partial x_j} + \Pi_{q_{gp}} - \alpha_p \rho_p \varepsilon_{gp}$$

Correlation velocity fluctuation gas-particles

$$\left\langle u'_{g,i} u'_{p,j} \right\rangle = -\nu^t_{gp} \left[\frac{\partial U_{g,i}}{\partial x_j} + \frac{\partial U_{p,j}}{\partial x_i} \right] + \frac{1}{3} \left[q_{gp} + \nu^t_{gp} \frac{\partial U_{g,m}}{\partial x_m} + \nu^t_{gp} \frac{\partial U_{p,m}}{\partial x_m} \right] \delta_{ij}$$

Dissipation

$$\varepsilon_{gp} = \frac{q_{gp}}{\tau^t_{gp}}$$

Turbulent viscosity $\nu^t_{gp} = \frac{1}{3} q_{gp} \tau^t_{gp}$

Influence of particle on correlation fluid particle velocity fluctuation

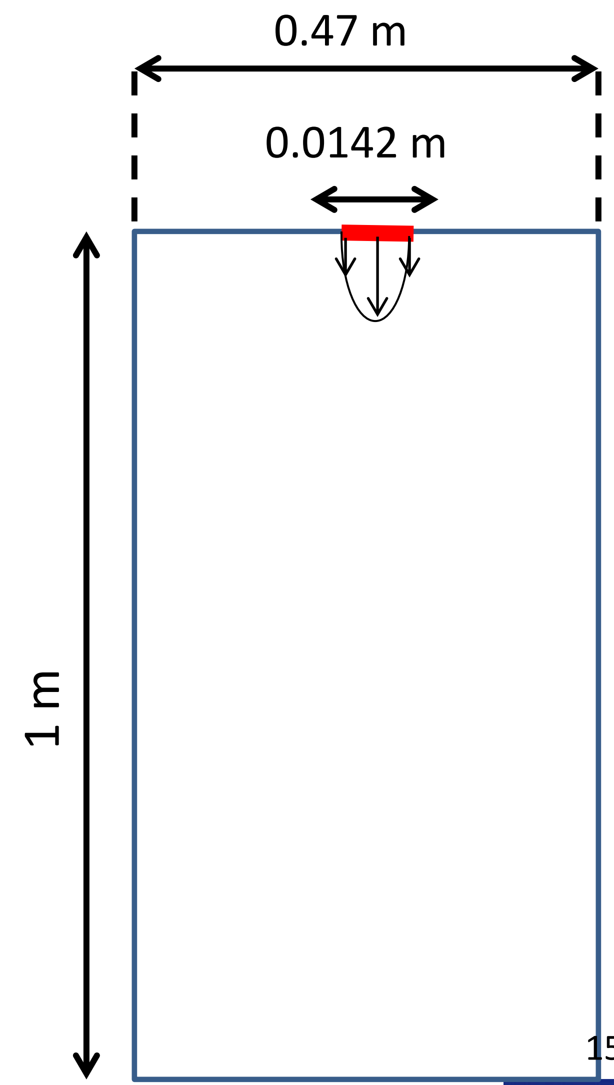
$$\Pi_{q_{gp}} = -\frac{\alpha_p \rho_p}{\tau^F_{gp}} \left[\left(1 + \frac{\alpha_p \rho_p}{\alpha_g \alpha_g} \right) q_{gp} - 2k - 2 \frac{\alpha_p \rho_p}{\alpha_g \alpha_g} q_p^2 \right]$$

[1]Boëlle, A., Balzer, G., Simonin, O., 1995. ASME FED, Gas–Solid Flow 228. 9–18.

III. Numerical simulation with NEPTUNE_CFD

Geometry

Geometry configuration	Nozzle diameter	0.0142 m
	Chamber test dimensions	0.47 m x 0.47 m x 1 m
Gas properties (air)	Density	1.18 kg/m^3
	Viscosity	1.85e-05 Pa.s
Particles properties (glass beads)	Density	2500 kg/m^3
	Diameters	25 µm and 70 µm
Particle mass loading	Monosized particle	1
	Binary mixture	0.5/class

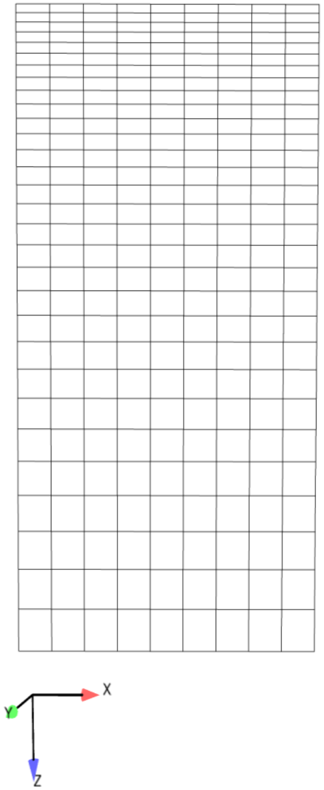


Mesh

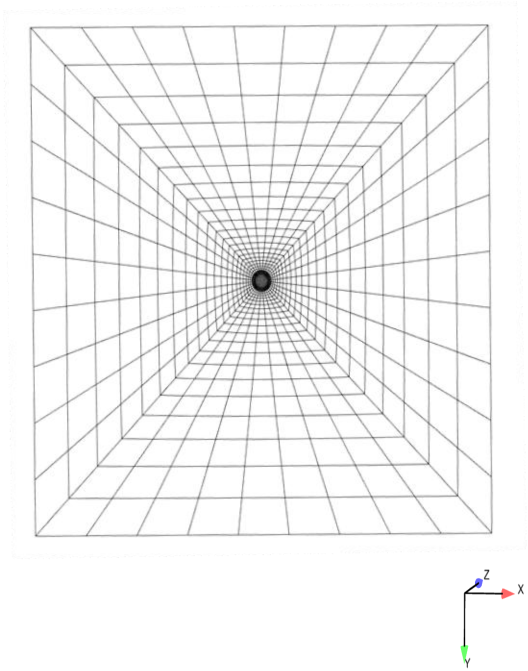
3D Structured Mesh

Number of cells : 61,950

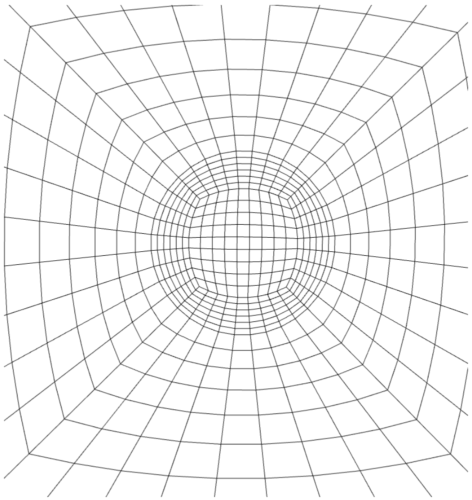
Mesh dimension: 0.47 m x 0.47 m x 1 m



Front view



Top view



Zoom at inlet region

$$\Delta x_{\min} \approx 0.001m$$
$$\Delta x_{\max} \approx 0.05m$$
$$\Delta y_{\min} \approx 0.001m$$
$$\Delta y_{\max} \approx 0.05m$$
$$\Delta z_{\min} \approx 0.04m$$
$$\Delta z_{\max} \approx 0.12m$$

Boundary conditions

Mean Velocity:

- Gas phase: interpolated from experimental data
- Particulate phases: interpolated from experimental data

Mean agitation:

k-ε model

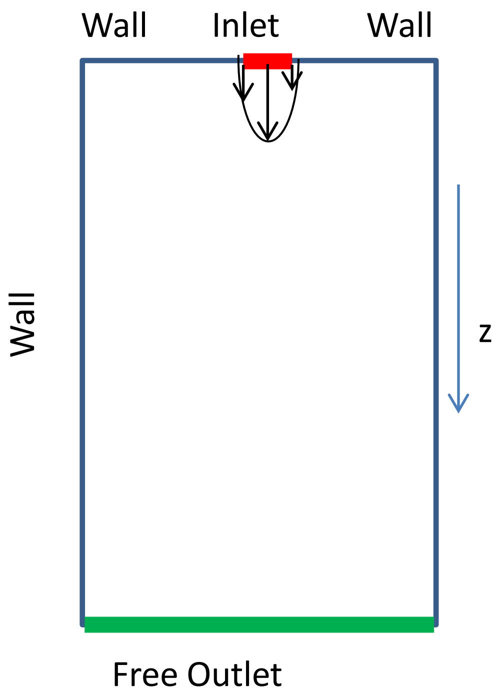
$$k = \frac{1}{2}\left[u'^2_{g,z} + 2u'^2_{g,x}\right]$$

$$\varepsilon = C_\mu \frac{k^{1.5}}{l_m} \qquad l_m = 0.03D \qquad C_\mu = 0.09$$

$q_p - q_{gp}$ model

$$q_p^2 = \frac{1}{2}\left[u'^2_{p,z} + 2u'^2_{p,x}\right]$$

$$q_{gp} = \frac{1}{2} q_p^2$$ (Tchen's hypothesis)



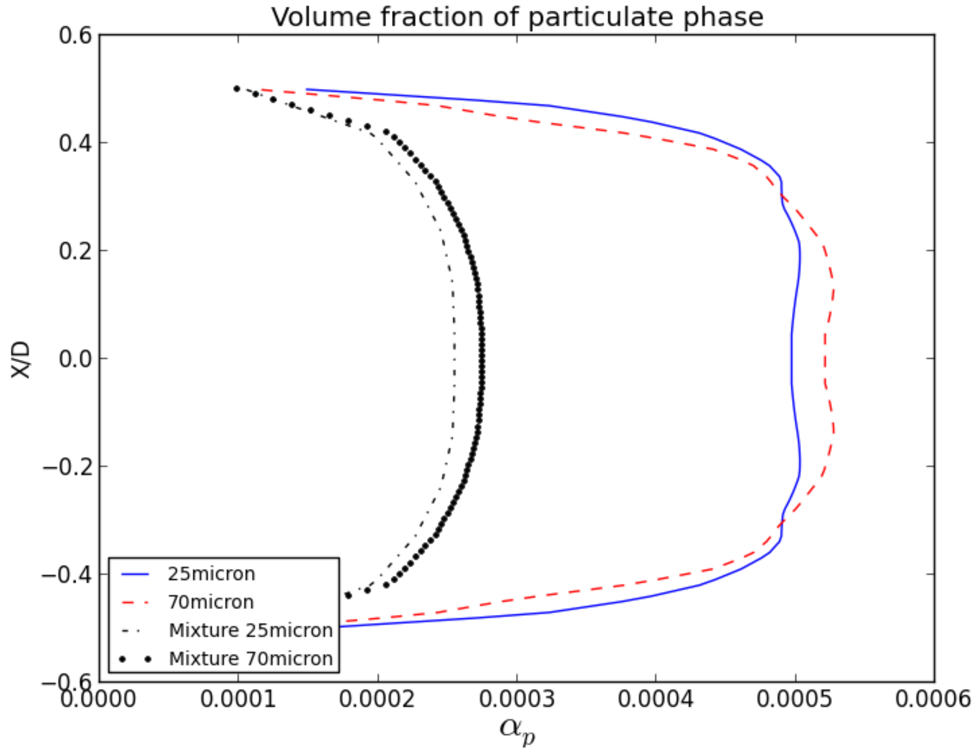
Boundary conditions

Particle mass loading for monodisperse case

$$m = \frac{\int_{A_c} \alpha_p \rho_p U_p dA_c}{\int_{A_c} (1-\alpha_p)\rho_g U_g dA_c}$$

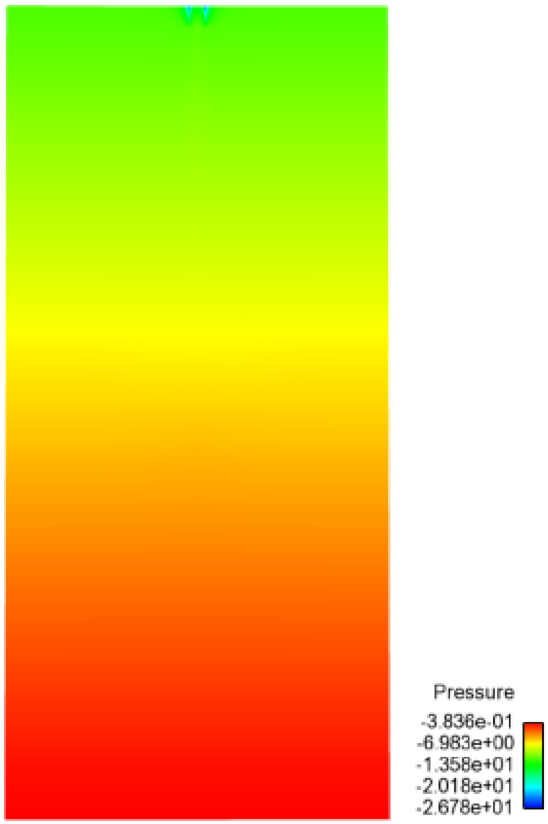
Volume fraction of particulate phase

$$\alpha_p = \frac{m\rho_g U_{g,z}}{m\rho_g U_{g,z} + \rho_p U_{p,z}}$$

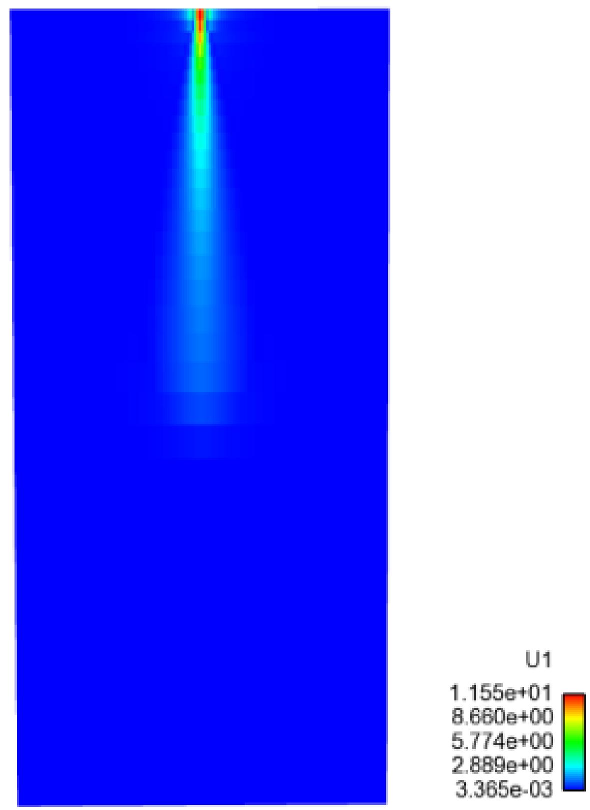


For 25 µm particles case and 70 µm particles case	$\alpha_p \approx 5\times10^{-4}$
For binary mixture case.	$\alpha_{p,25} \approx 2.5\times10^{-4}$ $\alpha_{p,70} \approx 2.5\times10^{-4}$

Numerical results- Single phase flow

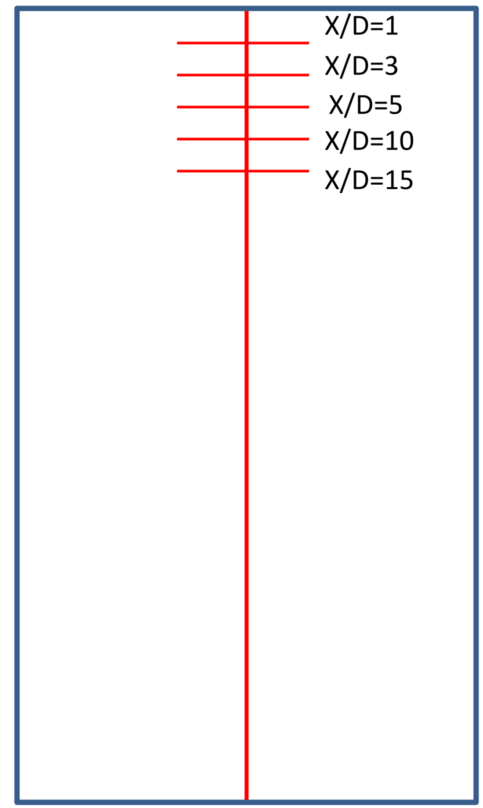


Relative pressure field



Velocity field of gas phase

Radial profils

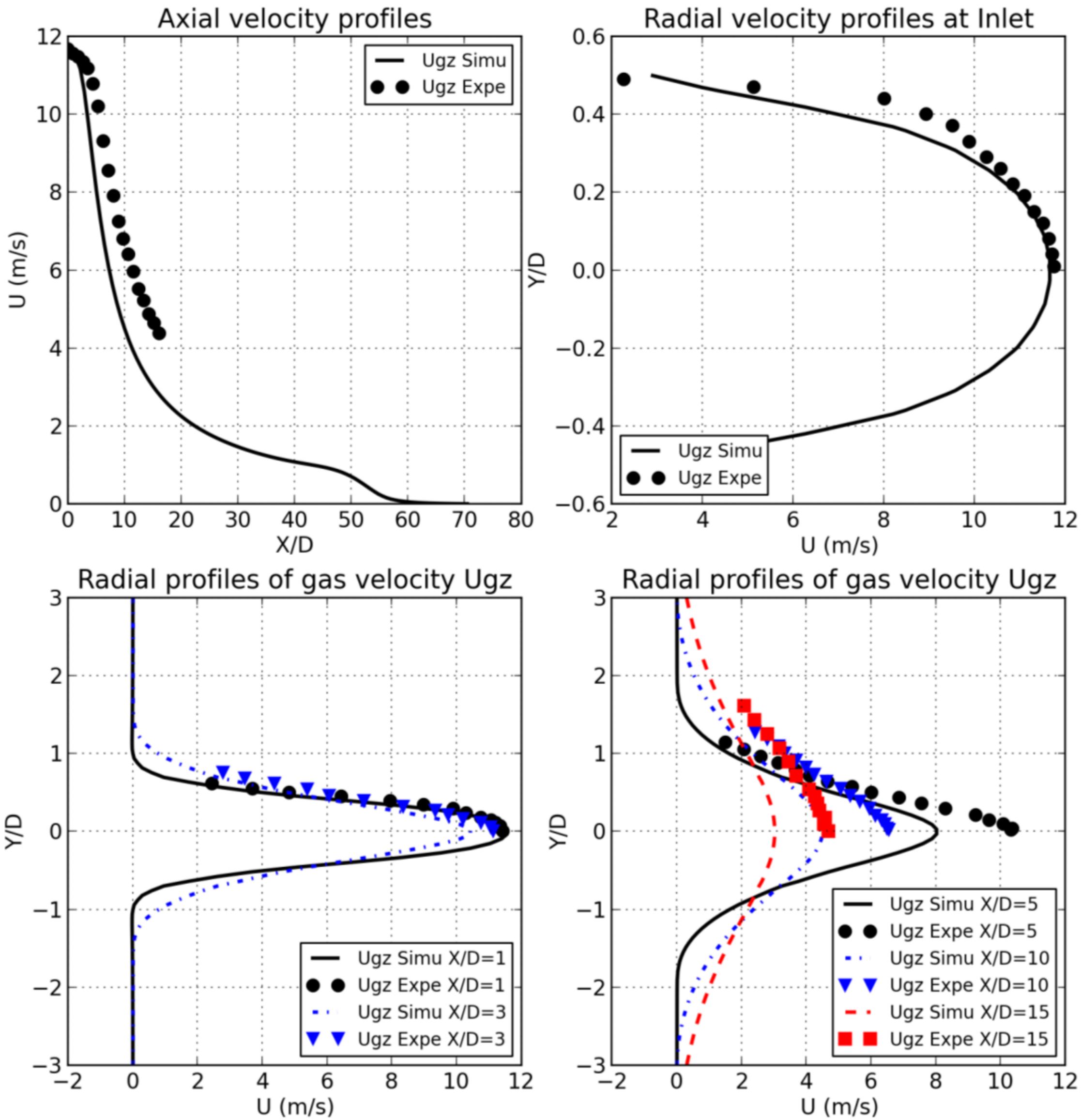


Axial profil

D: nozzle diameter

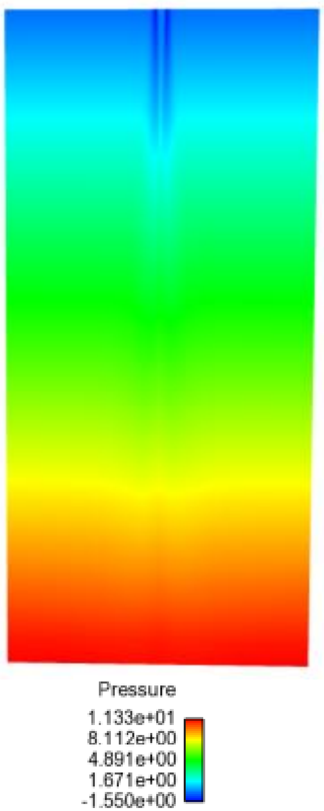
Physical time: 2s. Established regime

Numerical results- Single phase flow

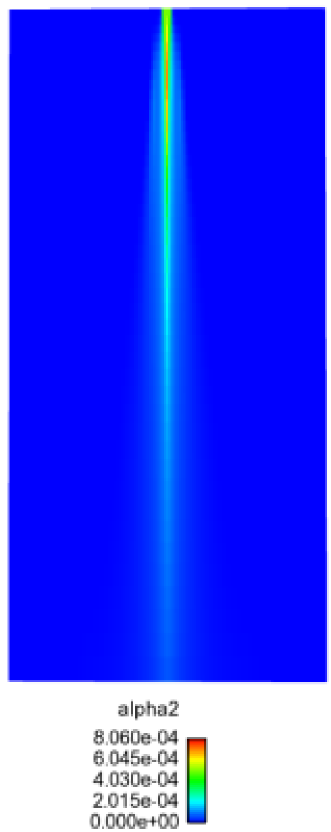


Ugz: axial component of gas velocity

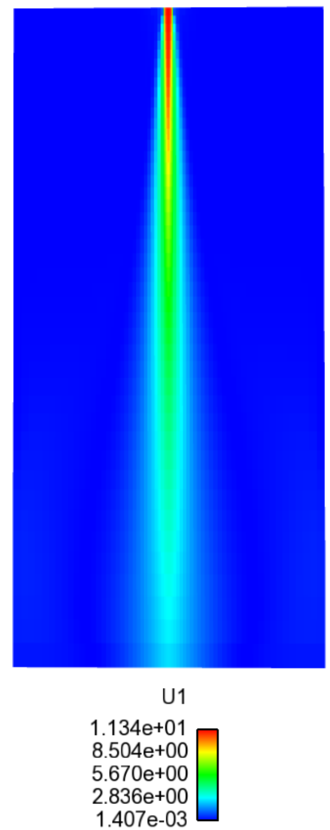
Numerical results- Two-phase flow with 25 µm particles



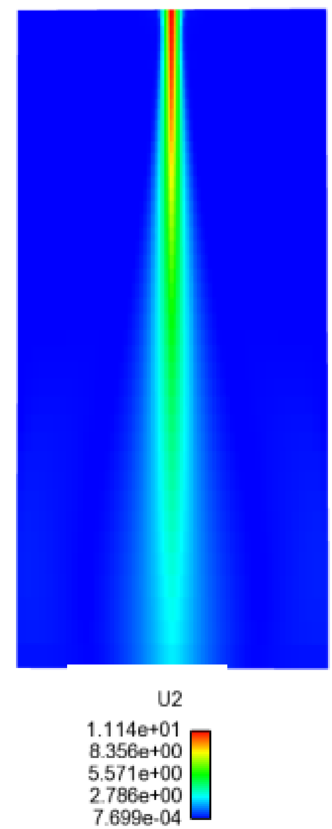
Relative pressure field



Volume fraction field of particulate phase

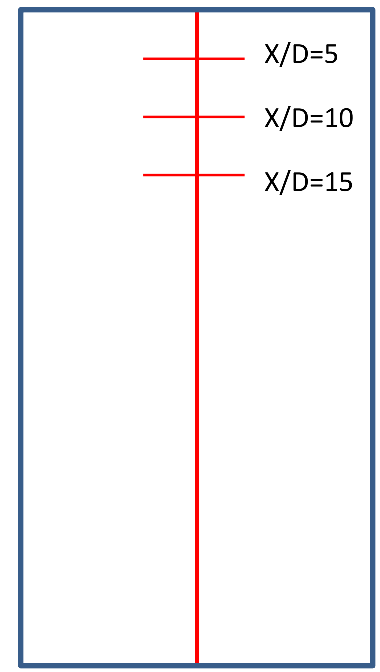


Velocity field of gas phase



Velocity field of particulate phase

Radial profiles

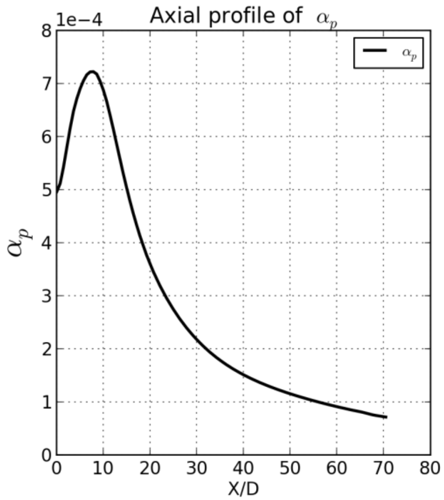


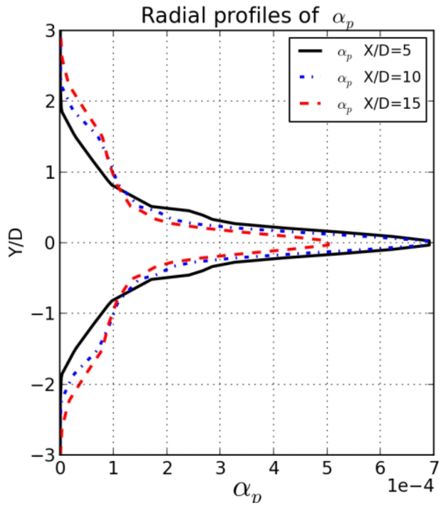
Axial profile

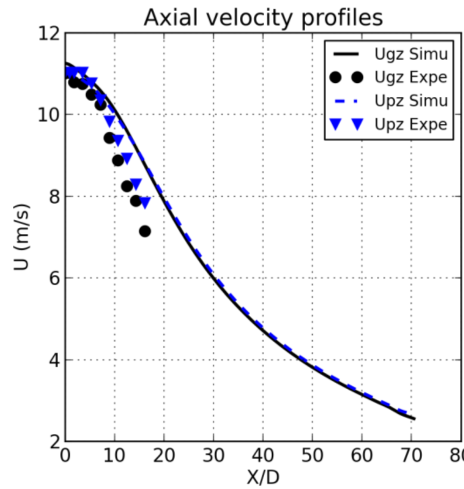
D: nozzle diameter

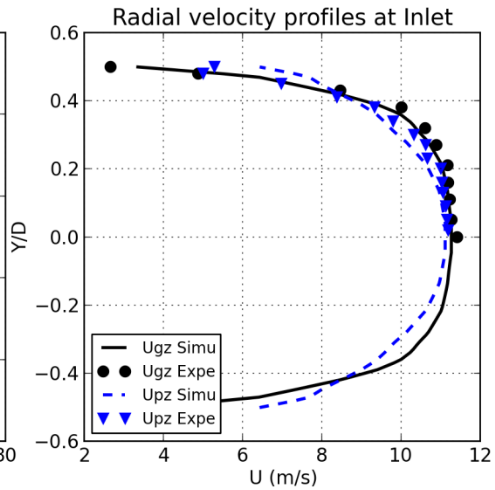
Physical time: 2s. Established regime

Numerical results- Two-phase flow with 25 µm particles

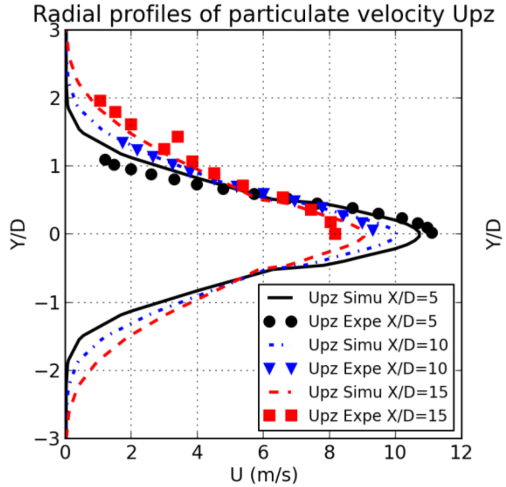


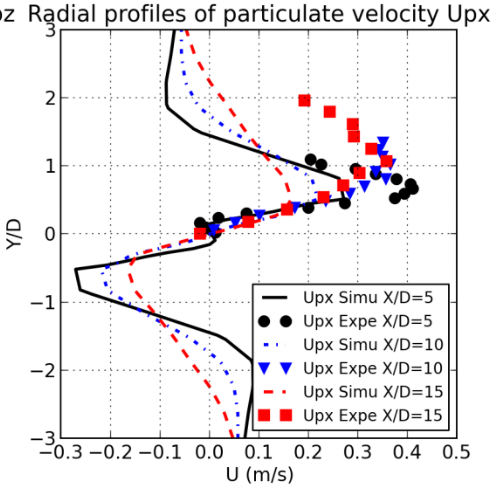






➔Turbophoresis phenomenon

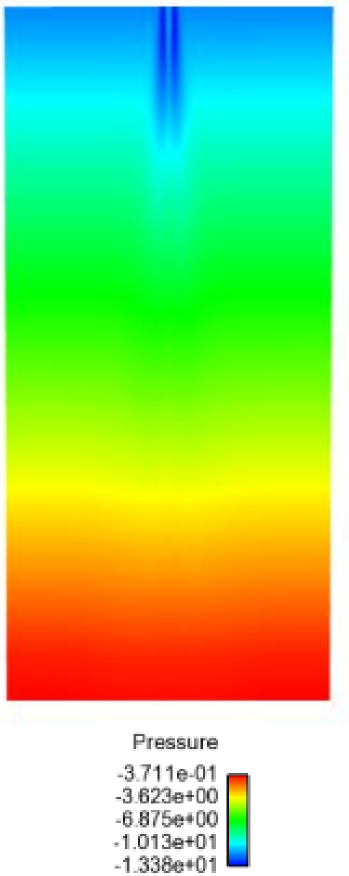




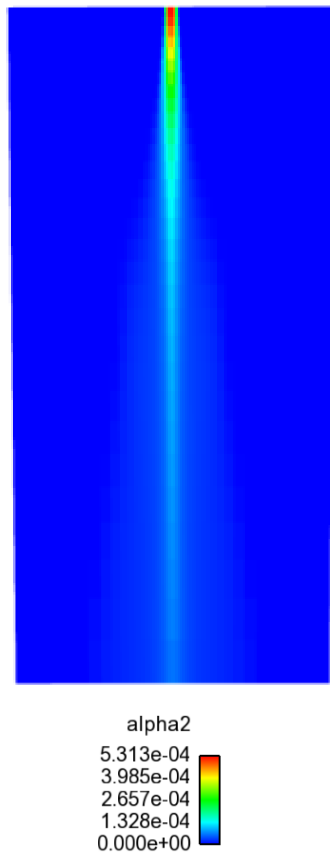
α_p volume fraction of particulate phase

Ugz: axial component of gas velocity
Upz: axial component of particulate velocity
Upx: radial component of particulate velocity

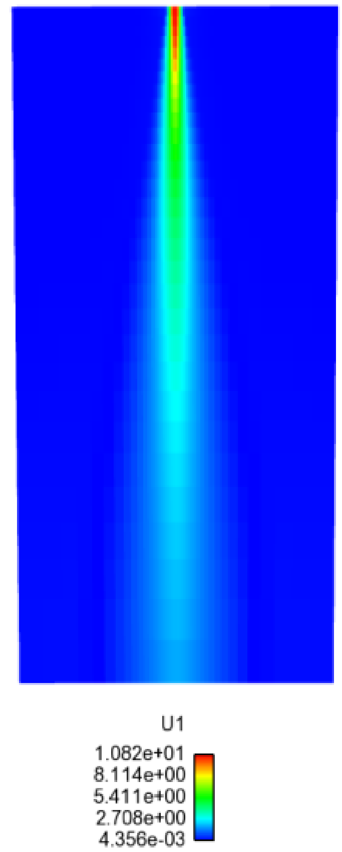
Numerical results- Two-phase flow with 70 µm particles



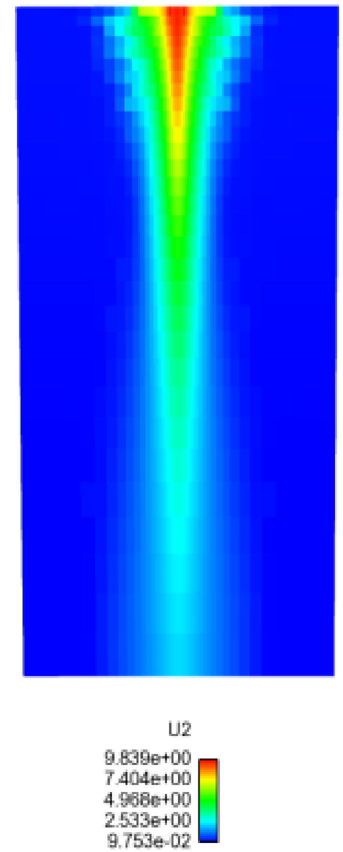
Relative pressure field



Volume fraction field of particulate phase

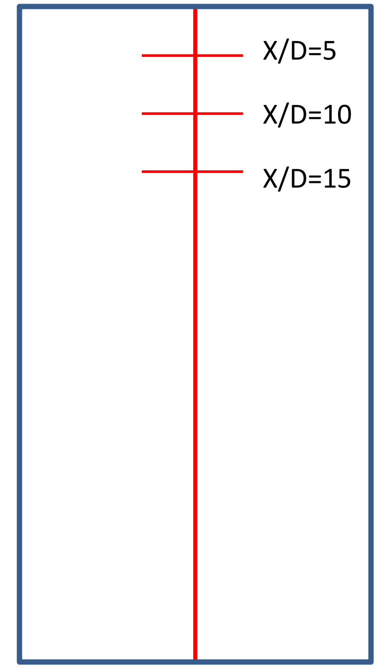


Velocity field of gas phase



Velocity field of particulate phase

Radial profiles

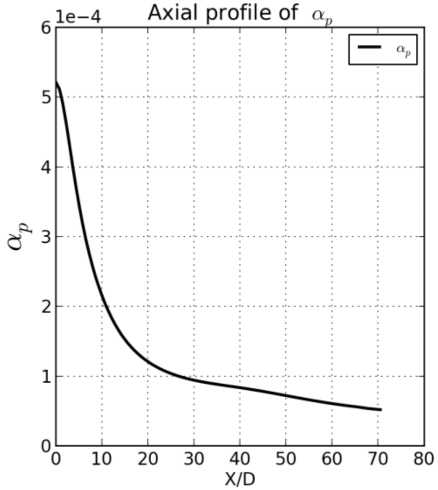


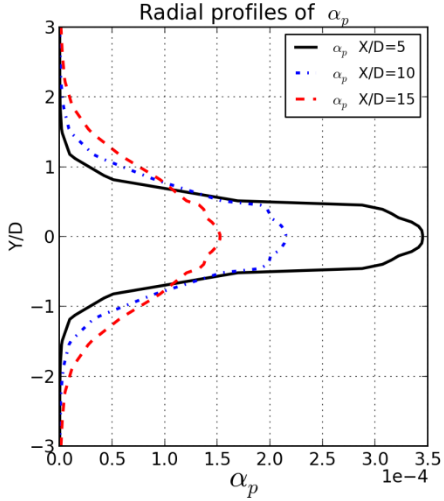
Axial profile

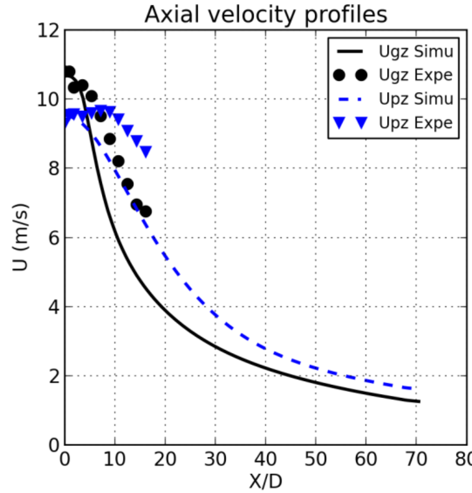
D: nozzle diameter

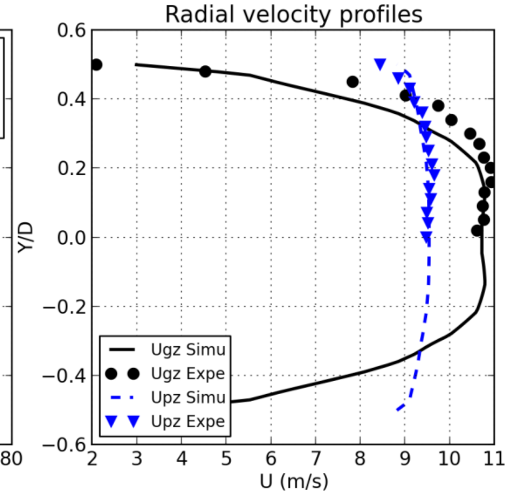
Physical time: 2s. Established regime

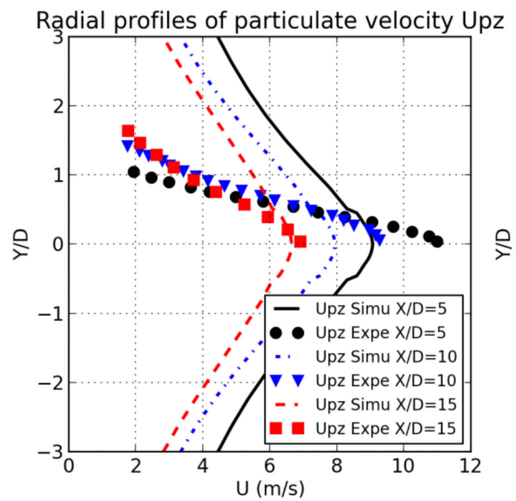
Numerical results- Two-phase flow with 70 µm particles

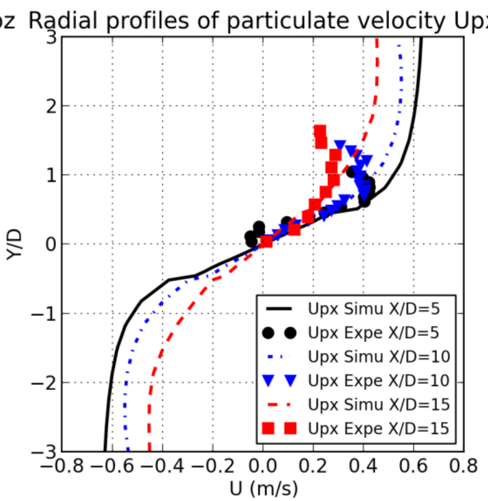












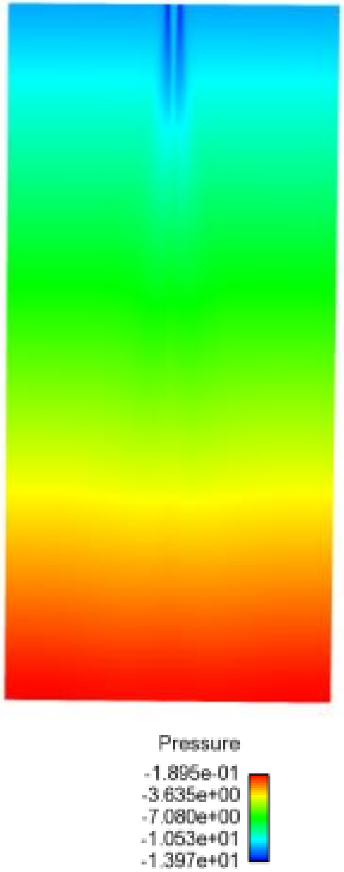
α_p volume fraction of particulate phase

Ugz: axial component of gas velocity

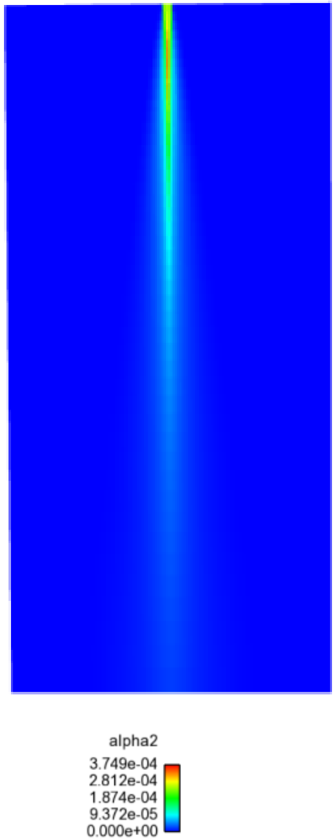
Upz: axial component of particulate velocity

Upx: radial component of particulate velocity

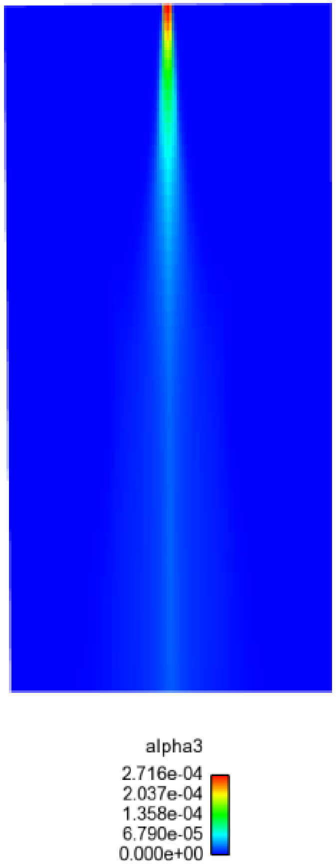
Numerical results- Two-phase flow with binary mixture



Relative pressure field



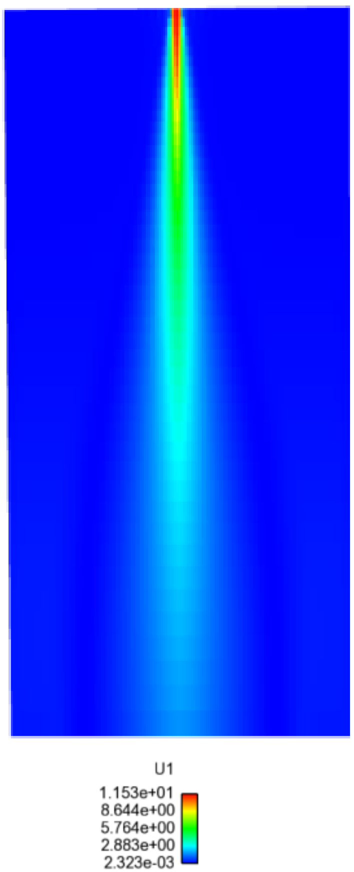
Volume fraction field of 25 µm particulate phase



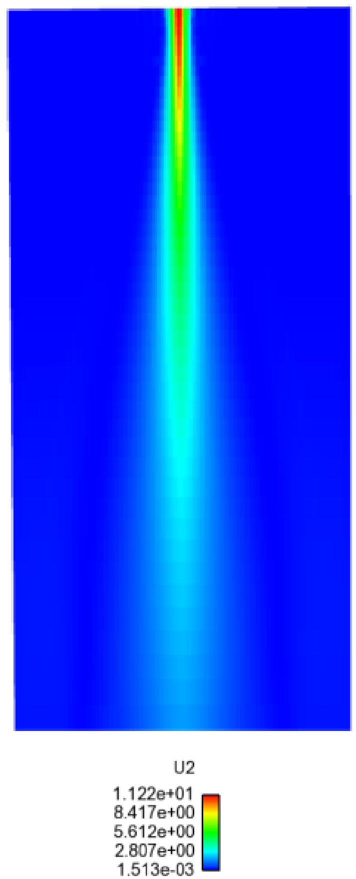
Volume fraction field of 70 µm particulate phase

Physical time: 2s. Established regime

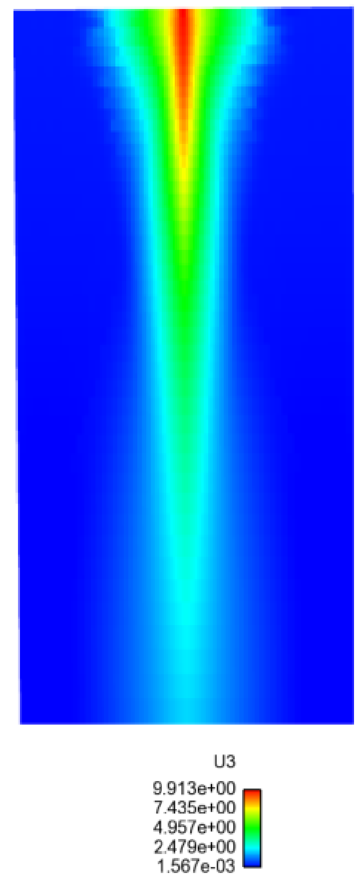
Numerical results- Two-phase flow with binary mixture



Velocity field of gas phase

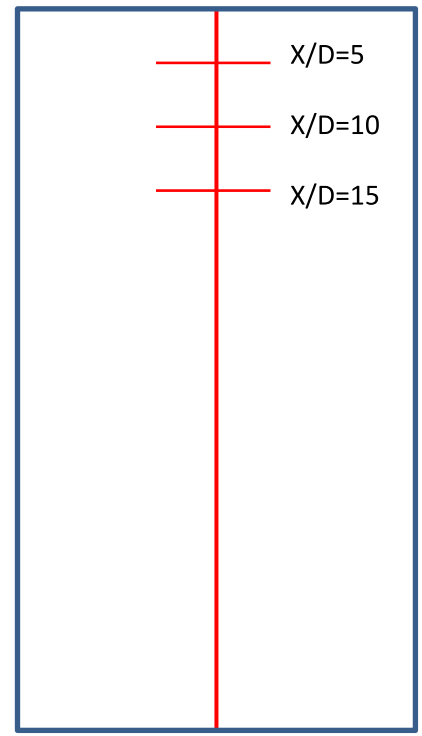


Velocity field of 25 µm particulate phase



Velocity field of 70 µm particulate phase

Radial profiles

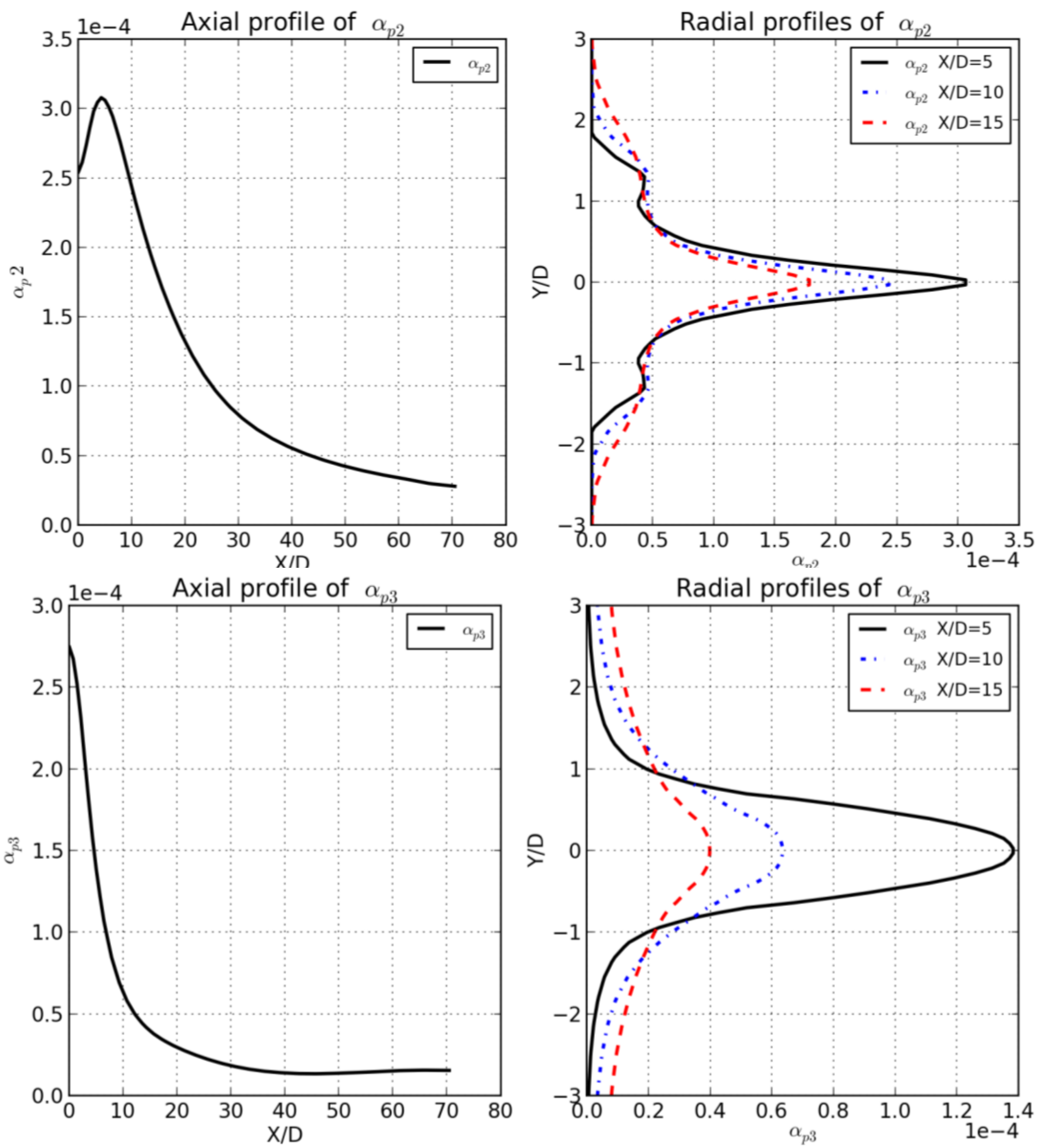


Axial profile

D: nozzle diameter

Physical time: 2s. Established regime

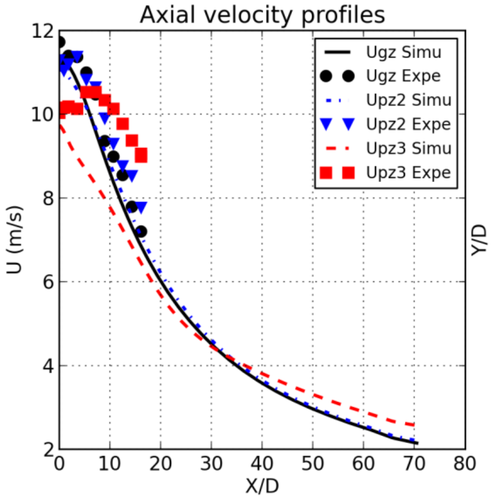
Numerical results- Two-phase flow with binary mixture

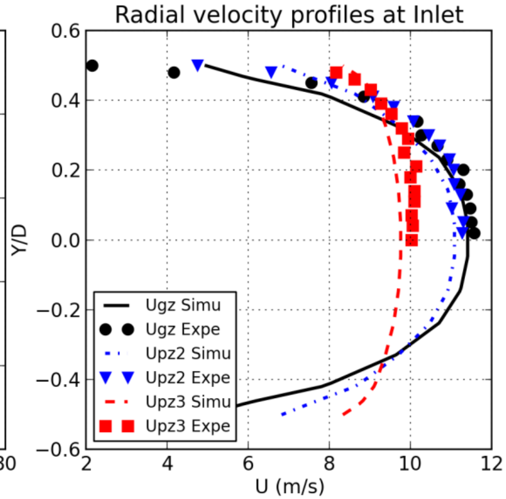


α_{p2} volume fraction of 25 µm particulate phase

α_{p3} volume fraction of 70 µm particulate phase

Numerical results- Two-phase flow with binary mixture





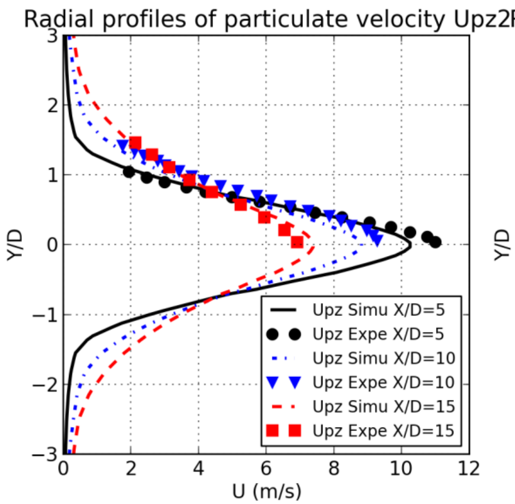
Ugz: axial component of gas velocity

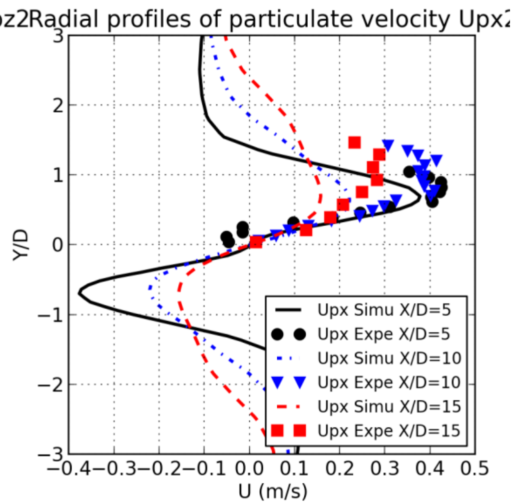
Upz2: axial component of particulate velocity of 25 µm particle

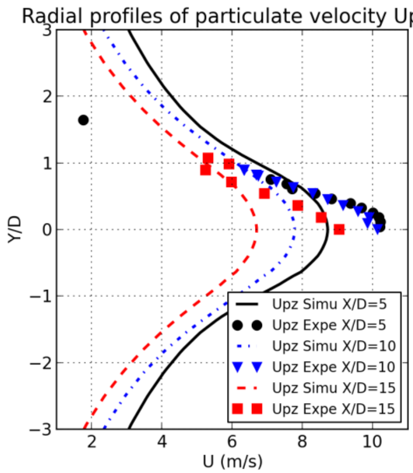
Upx2: radial component of particulate velocity of 25 µm particle

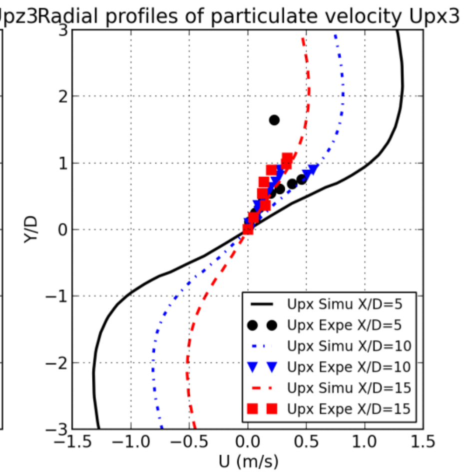
Upz3: axial component of particulate velocity of 70 µm particle

Upx3: radial component of particulate velocity of 70 µm particle









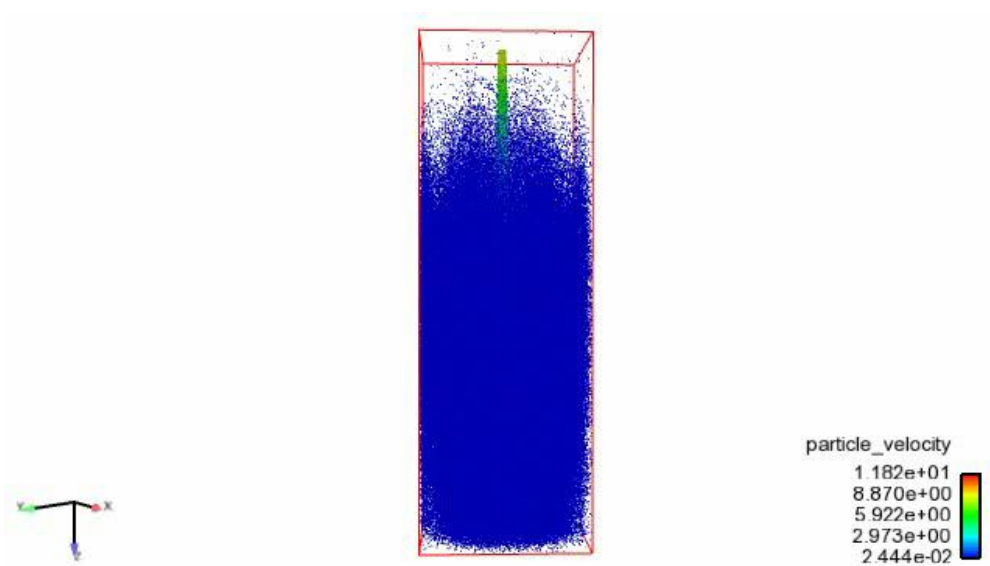
IV. Conclusions and perspectives

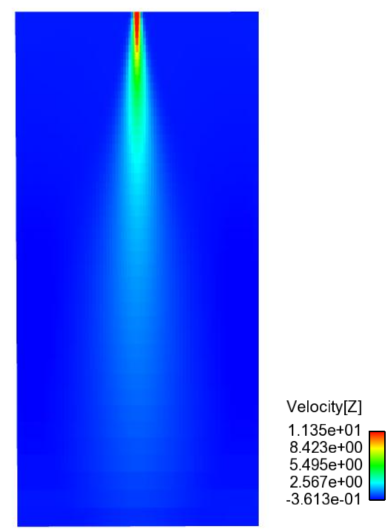
Conclusions

- Good agreement between numerical simulation and experimental results is obtained
- Some differences are mainly observed for 70 µm particle for monodisperse and binary mixture cases.

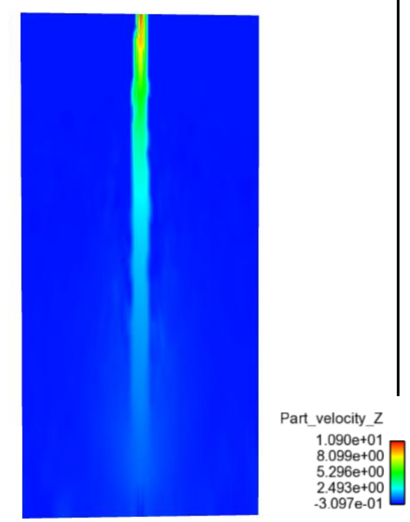
Outlook

- The numerical simulation with Code_Saturne is on going.
- The modelling of brownian motion and agglomeration for nanoparticle will be implemented to numerical tools Neptune_CFD and/or Code_Saturne.





Velocity of gas phase



Velocity projected on Eulerien mesh of particulate phase.

Thank you for your attention!