ROCKY

DEM AND CFD COUPLING

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OUTLINE

- DEM-CFD Coupling Formulation
- Validation cases

DEM

$$m_p \frac{d\mathbf{v}_p}{dt} = \boxed{\mathbf{F}_c} + \boxed{\mathbf{F}_{f\rightarrow p}} + m_p \mathbf{g}$$

particle-particle and particle-wall contact forces

fluid-particle interaction

$$\mathbf{F}_{f\rightarrow p} = \boxed{\mathbf{F}_{\mathrm{D}} + \mathbf{F}_{\nabla p} + \mathbf{F}_{\mathrm{L}} + \mathbf{F}_{\mathrm{VM}}} + \mathbf{F}_{\mathrm{others}}$$

Currently available in Rocky

Euler's Equations: $\mathbf{I}_p \frac{d\boldsymbol{\omega}_p}{dt} - \left(\mathbf{I}_p \cdot \boldsymbol{\omega}_p\right) \times \boldsymbol{\omega}_p = \mathbf{T}_p + \mathbf{T}_p^{f\rightarrow p}$

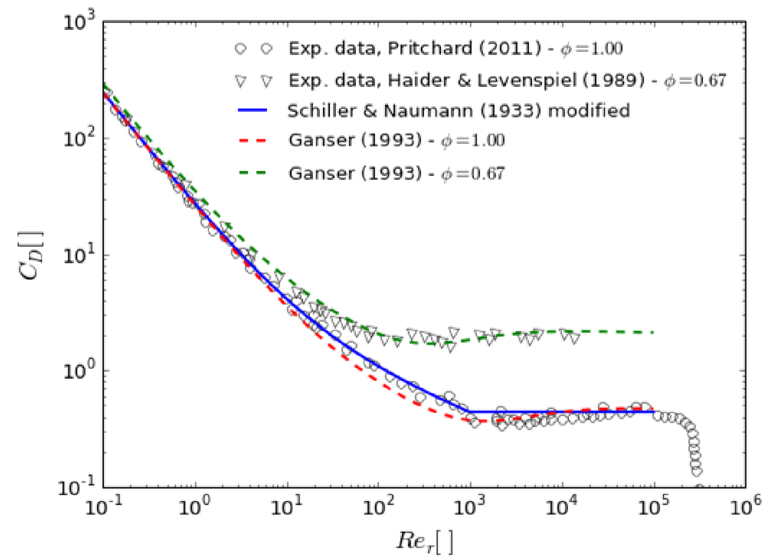
DRAG MODELS

$$C_D = \frac{\mathbf{F}_\mathrm{D}}{\frac{1}{2}\rho_f A' \left|\mathbf{u}_f - \mathbf{v}_p\right| (\mathbf{u}_f - \mathbf{v}_p)}$$

- Dilute flows
  - Schiller & Naumann (1933)
  - DallaValle (1948)
  - Haider & Levenspiel (1989)
  - Ganser (1993)

Spherical particles

Takes into account shape



- Dense flows
  - Wen & Yu (1966)
  - Ergun (1958)
  - Huilin & Gidaspow (2003)
  - Di Felice (1994)

FLUID-PARTICLES INTERACTION FORCES

- Virtual mass force

$$\mathbf{F}_{\mathrm{VM}} = C_{\mathrm{VM}} \rho_f V_p \mathbf{a}_r$$

- Available virtual mass models:
  - Constant
  - Ishii & Mishima (1984)
  - Paladino (2005)

- Lift force

$$C_L = \frac{\mathbf{F}_L}{\rho_f V_p \mathbf{u}_r \times (\nabla \times \mathbf{u})}$$

- Available lift models:
  - Saffman (1968)
  - Mei (1992)

PARTICLE HEAT TRANSFER

$$m_p c_p \frac{dT_p}{dt} = \boxed{q}$$

Convective fluid-particle heat transfer

contact heat transfer

$$m_p c_p \frac{\partial T_{av}(t)}{\partial t} = \boxed{A_p h\left(T_m(t) - T_p(R,t)\right)} - \boxed{A_p q''} + \boxed{V_p q'''}$$

Particle heat source

- For stardard (lumped) formulation: $T_p(R,t) \cong T_{av}(t)$

- For improved (lumped) formulation: $T_p\left(R,t\right) = \dfrac{8k_p T_{av}(t) + h(t) R T_{av}(t) - q''(t) R}{8k_p + h(t) R}$

PARTICLE HEAT TRANSFER

- Heat transfer coefficient based on Nusselt number:

$$Nu = \frac{hd_p}{k_f}$$

- Available Nusselt number correlations:
  - Ranz & Marschall (1952)
  - Whitaker (1972)
  - Gunn (1978)

Single particle

Fixed or fluidized beds

CFD

- Influence of particle on the fluid flow is taken into account by the volume fraction and momentum exchange force.

$$\frac{\partial}{\partial t}\left(\alpha_f \rho_f\right) + \nabla \cdot \left(\alpha_f \rho_f \mathbf{u}\right) = 0$$

$$\frac{\partial}{\partial t}\left(\alpha_f \rho_f \mathbf{u}\right) + \nabla \cdot \left(\alpha_f \rho_f \mathbf{u}\mathbf{u}\right) = -\alpha_f \nabla P + \alpha_f \nabla \cdot \tau_f + \alpha_f \rho_f \mathbf{g} - \boxed{\mathbf{F}^{p \to F}}$$

$$\boxed{\mathbf{F}^{p \to F} = \frac{\sum_{p=1}^{N} \boxed{\mathbf{F}_p^{F \to p}}}{V_{cell}}}$$

particle-fluid interaction

Calculated on DEM software

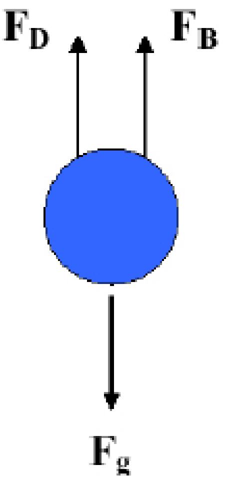
CASE 1 – FREE FALLING PARTICLE

- Free falling particle in water

$$m_p \frac{dv_z}{dt} = m_p\left(\rho_p - \rho_f\right) V_p g_z - \frac{1}{2}\rho_f C_D A v_{z_r}^2$$

- Schiller & Naumann drag correlation

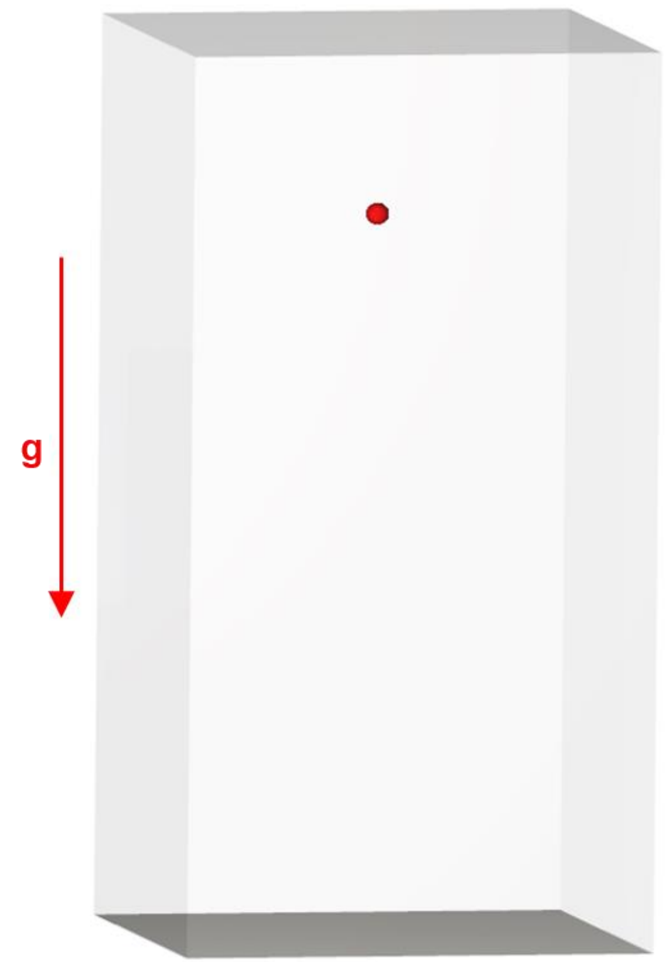
$$C_D = \max\left[\frac{24}{Re_p}\left(1 + 0.15 Re_p^{0.687}\right), 0.44\right]$$



CASE 1 – FREE FALLING PARTICLE

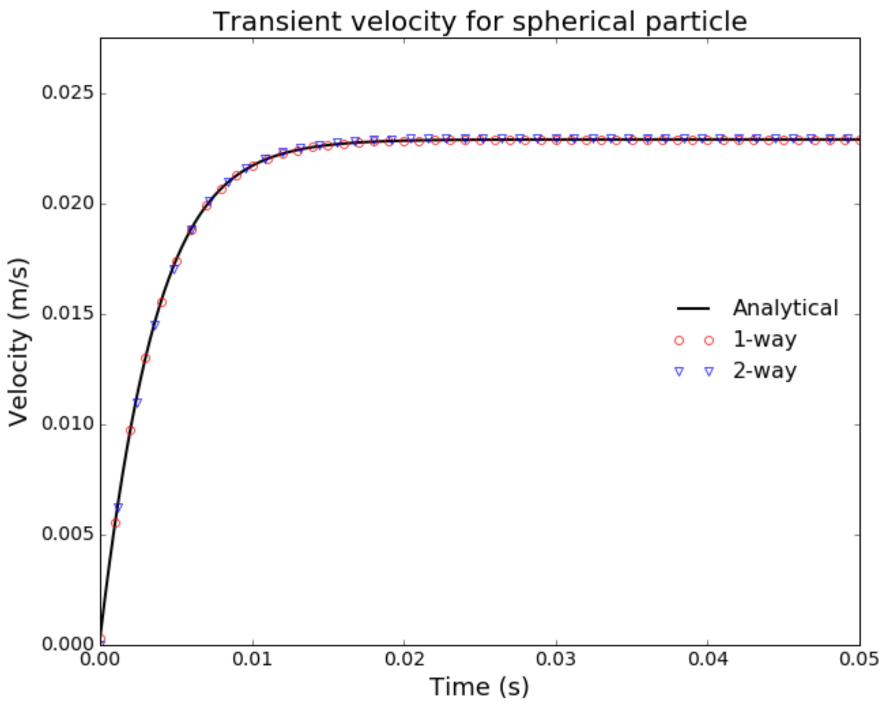
- Free falling particle
- Laminar flow

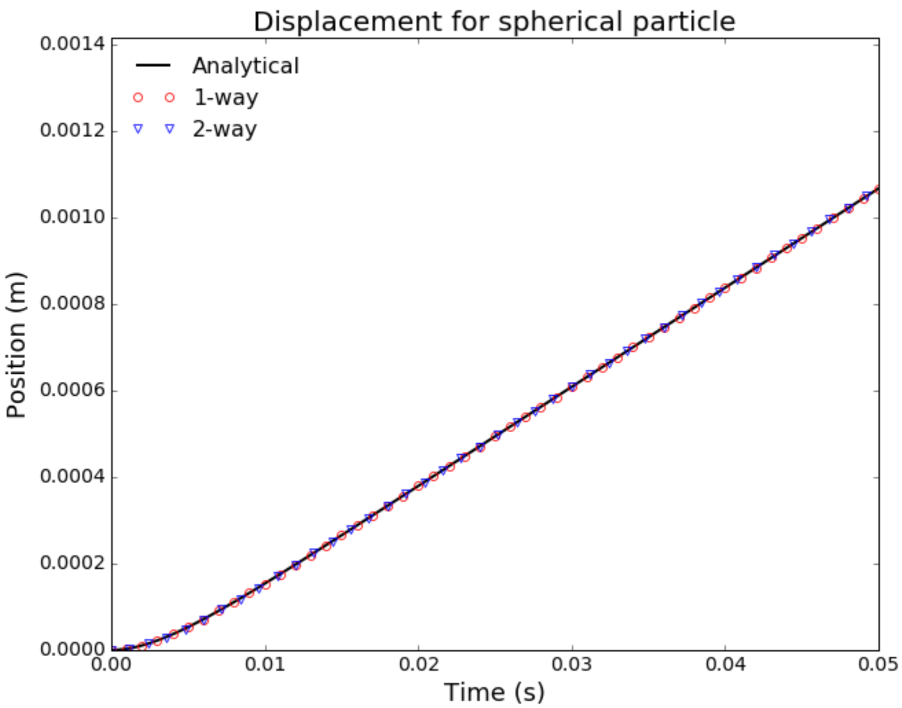
		Value	Unit
Domain	Dimensions	4x8x4	mm
	Mesh size	0.25	mm
Particle	Diameter	0.2	mm
	Density	2500	Kg/m^3
Water	Viscosity	0.001	Pa.s
	Density	1000	Kg/m^3



CASE 1 – FREE FALLING PARTICLE

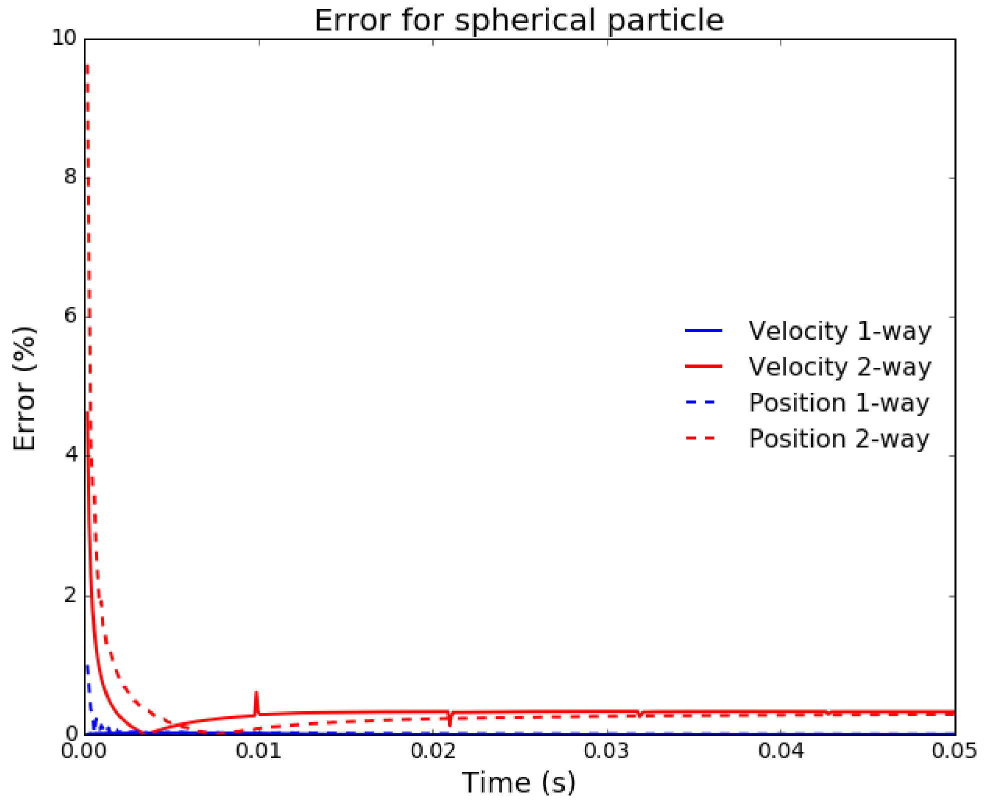
- Velocity and position





CASE 1 – FREE FALLING PARTICLE

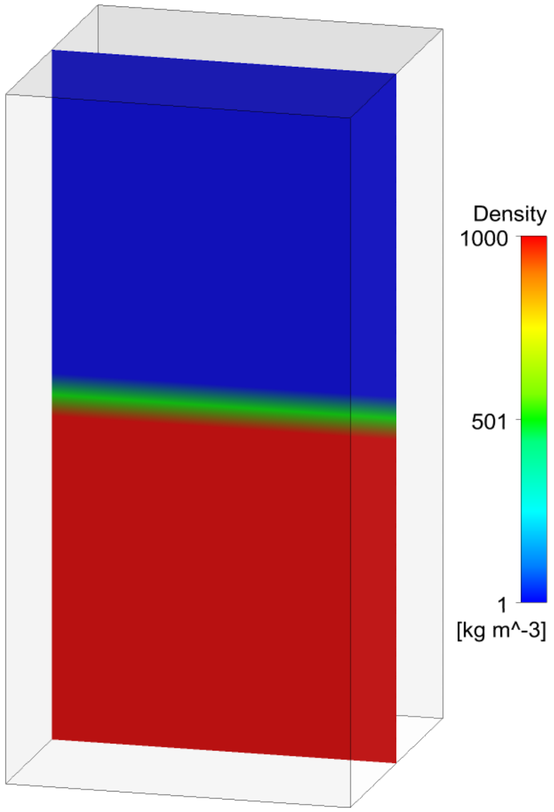
- Free falling particle



CASE 2 – FREE FALLING PARTICLE IN TWO-FLUIDS DOMAIN

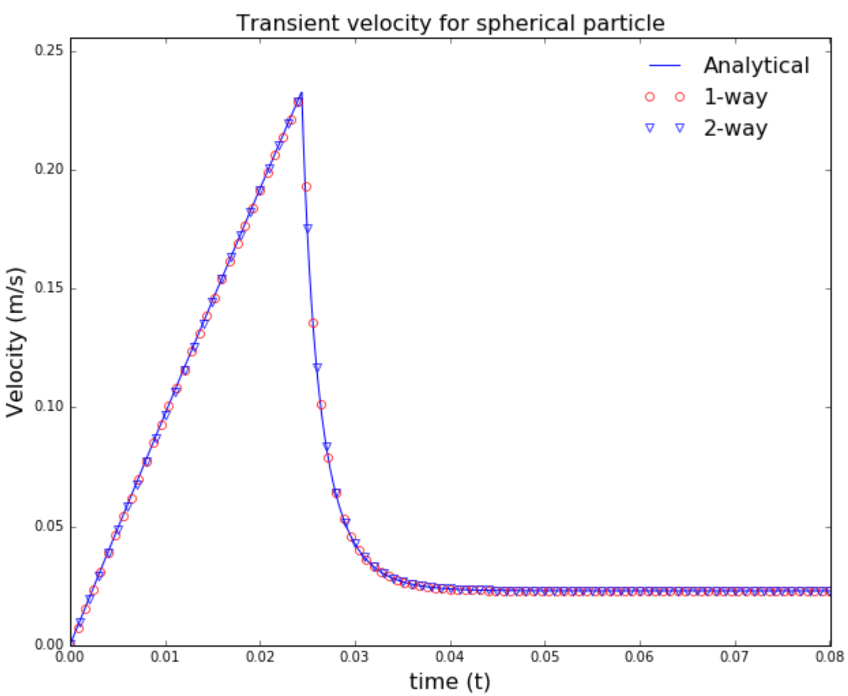
- Free falling particle in two-fluids domain

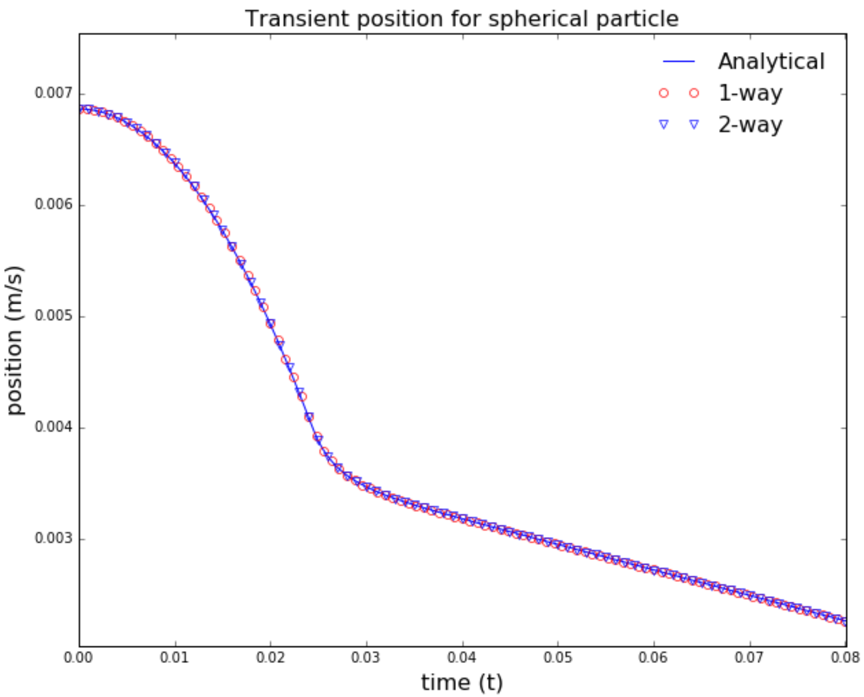
		Value	Unit
Domain	Dimensions	4x8x4	mm
	Mesh size	0.25	mm
Particle	Diameter	0.2	mm
	Density	2500	Kg/m^3
Air	Viscosity	0.00001	Pa.s
	Density	1	Kg/m^3
Water	Viscosity	0.001	Pa.s
	Density	1000	Kg/m^3



CASE 2 – FREE FALLING PARTICLE IN TWO-FLUIDS DOMAIN

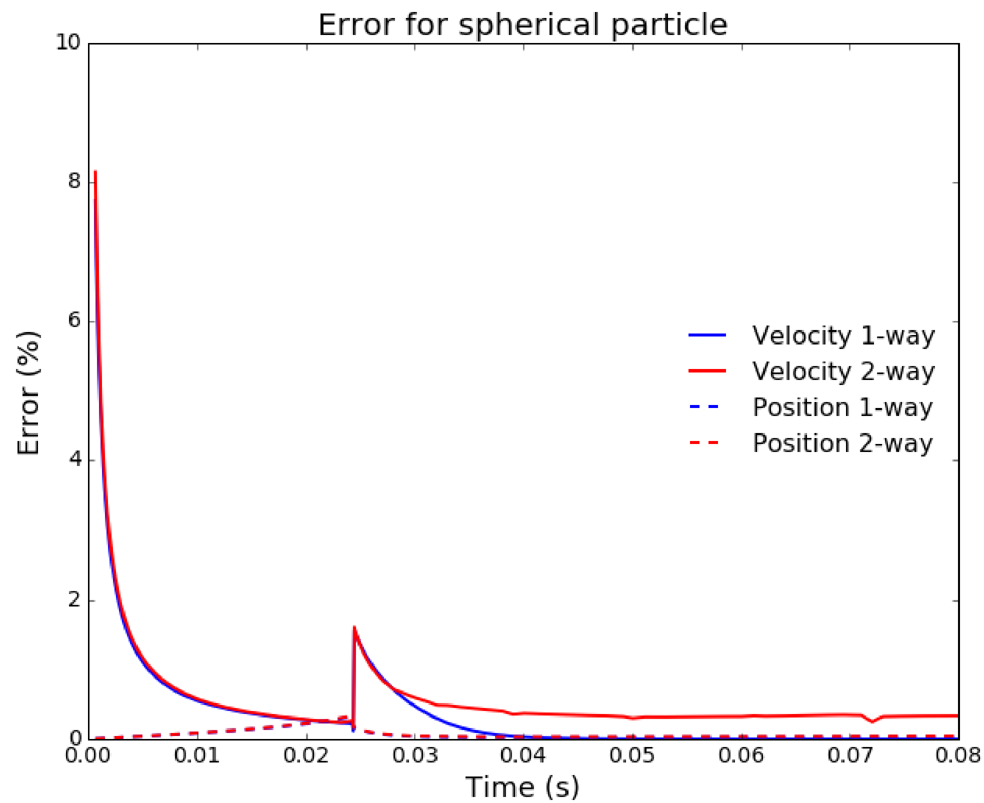
- Velocity and position



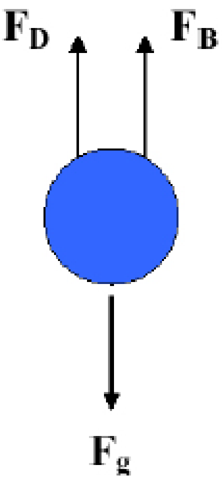


CASE 2 – FREE FALLING PARTICLE IN TWO-FLUIDS DOMAIN

- Free falling particle



CASE 3 – COOLING PARTICLE WITH STANDARD FORMULATION



- Cooling particle in water

$$m_p \frac{dv_z}{dt} = m_p \left(\rho_p - \rho_f\right) V_p g_z - \frac{1}{2} \rho_f C_D A v_{z_r}^2$$

- Schiller & Naumann drag correlation

$$C_D = \max\left[\frac{24}{Re_p}\left(1 + 0.15 Re_p^{0.687}\right), 0.44\right]$$

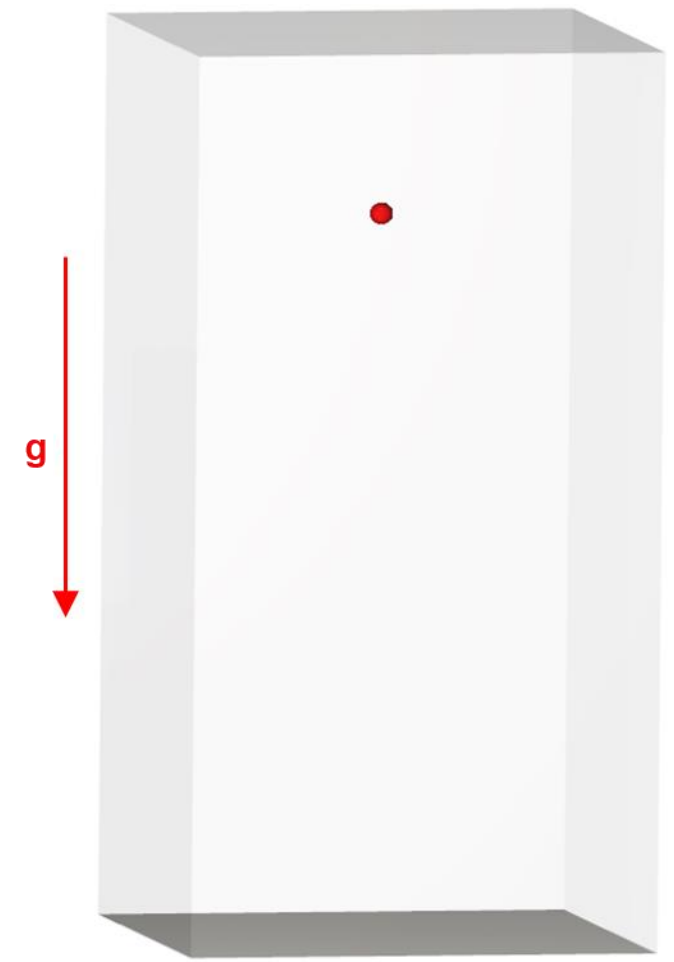
- Temperature variation as function of heat exchange with water

$$T_p = T_p^0 + \frac{q_{f\to p} \Delta t}{m_p c_p} \qquad q_{f\to p} = \left(\frac{Nu\, k_f}{d_p}\right) A_p \left(T_f - T_p^0\right)$$

- Whitaker and Ranz & Marshal correlation for Nusselt number

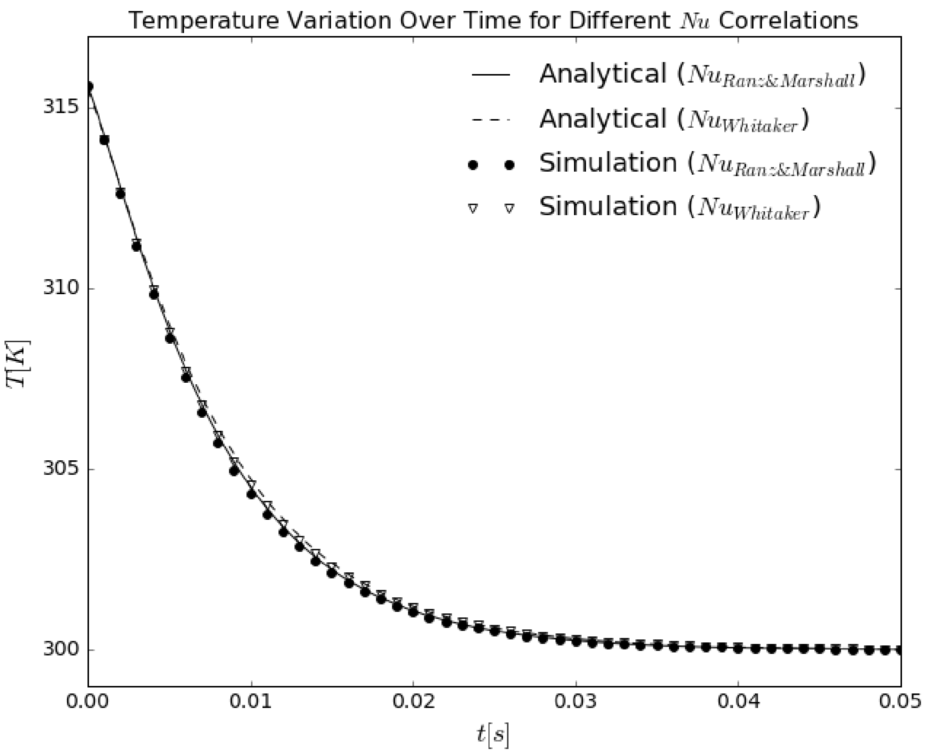
CASE 3 – COOLING PARTICLE WITH STANDARD FORMULATION

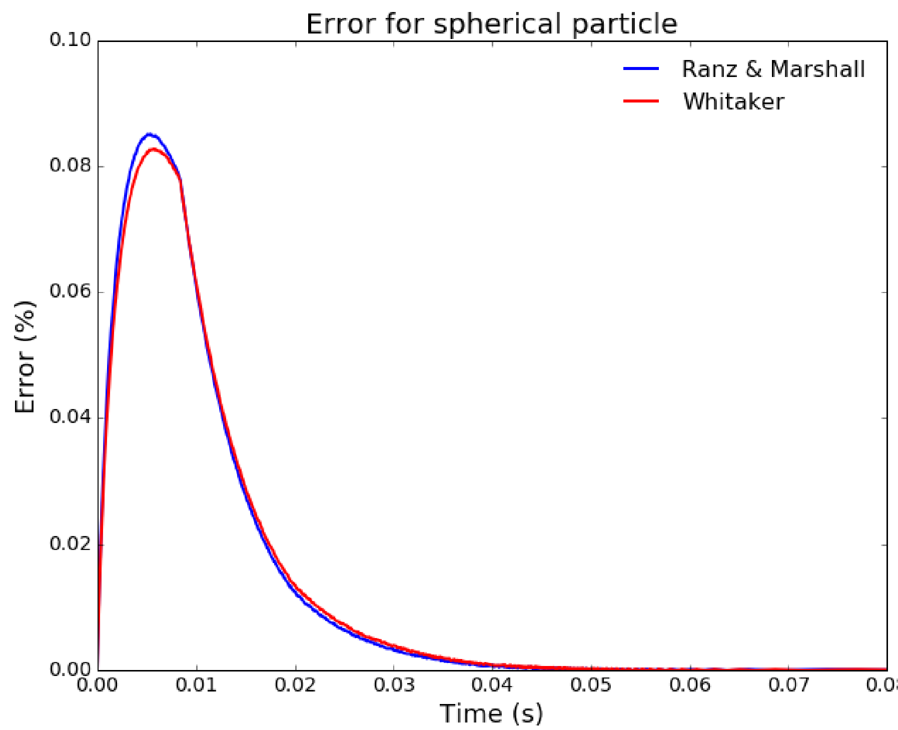
		Value	Unit
Domain	Dimensions	4x8x4	mm
	Mesh size	0.25	mm
Particle	Diameter	0.2	mm
	Density	2500	Kg/m^3
	Heat Capacity	1000	J/kg.K
	Thermal conductivity	100	W/m.K
	Initial temperature	500	K
Water	Viscosity	0.001	Pa.s
	Density	1000	Kg/m^3
	Heat Capacity	5000	J/kg.K
	Thermal conductivity	0.5	W/m.K
	Temperature	300	K



CASE 3 – COOLING PARTICLE WITH STANDARD FORMULATION

- Standard formulation
- Thermal conductivity = 100 W/m.K
  - Bi =0.01



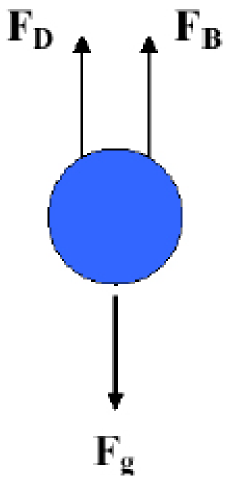


CASE 4 – COOLING PARTICLE WITH IMPROVED FORMULATION

- Cooling particle in water

$$m_p \frac{dv_z}{dt} = m_p \left(\rho_p - \rho_f\right) V_p g_z - \frac{1}{2} \rho_f C_D A v_{z_r}^2$$

- Schiller & Naumann drag correlation
- Ranz & Marshal correlation for Nusselt number

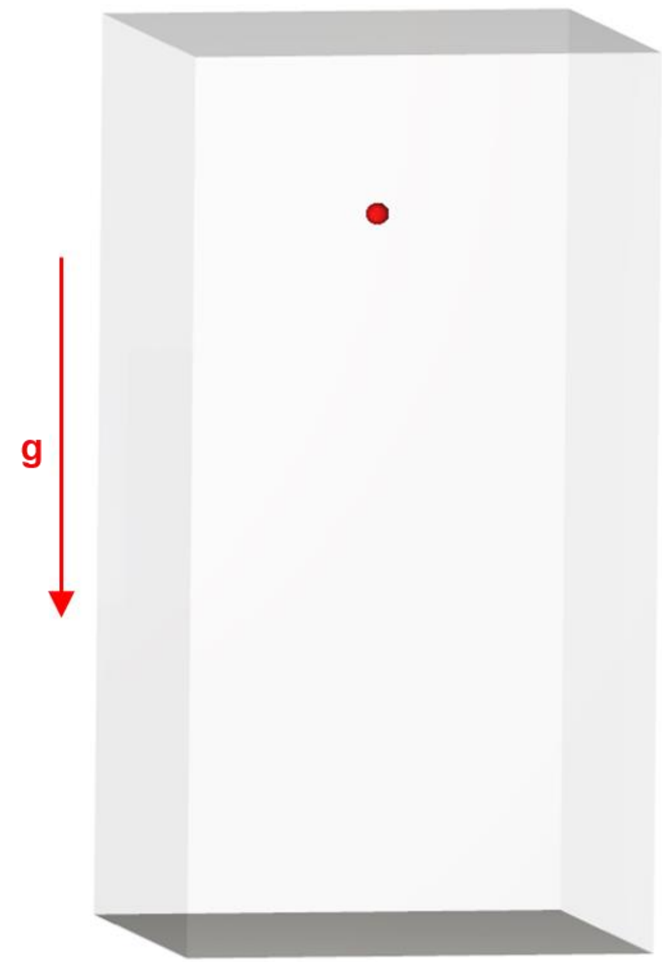


- Temperature variation as function of heat exchange with water

$$T_p = T_p^0 + \frac{q_{f \to p} \Delta t}{m_p c_p} \qquad q_{f \to p} = \left(\frac{Nu\, k_f}{d_p}\right) A_p \left(T_f - T_p^0\right)$$

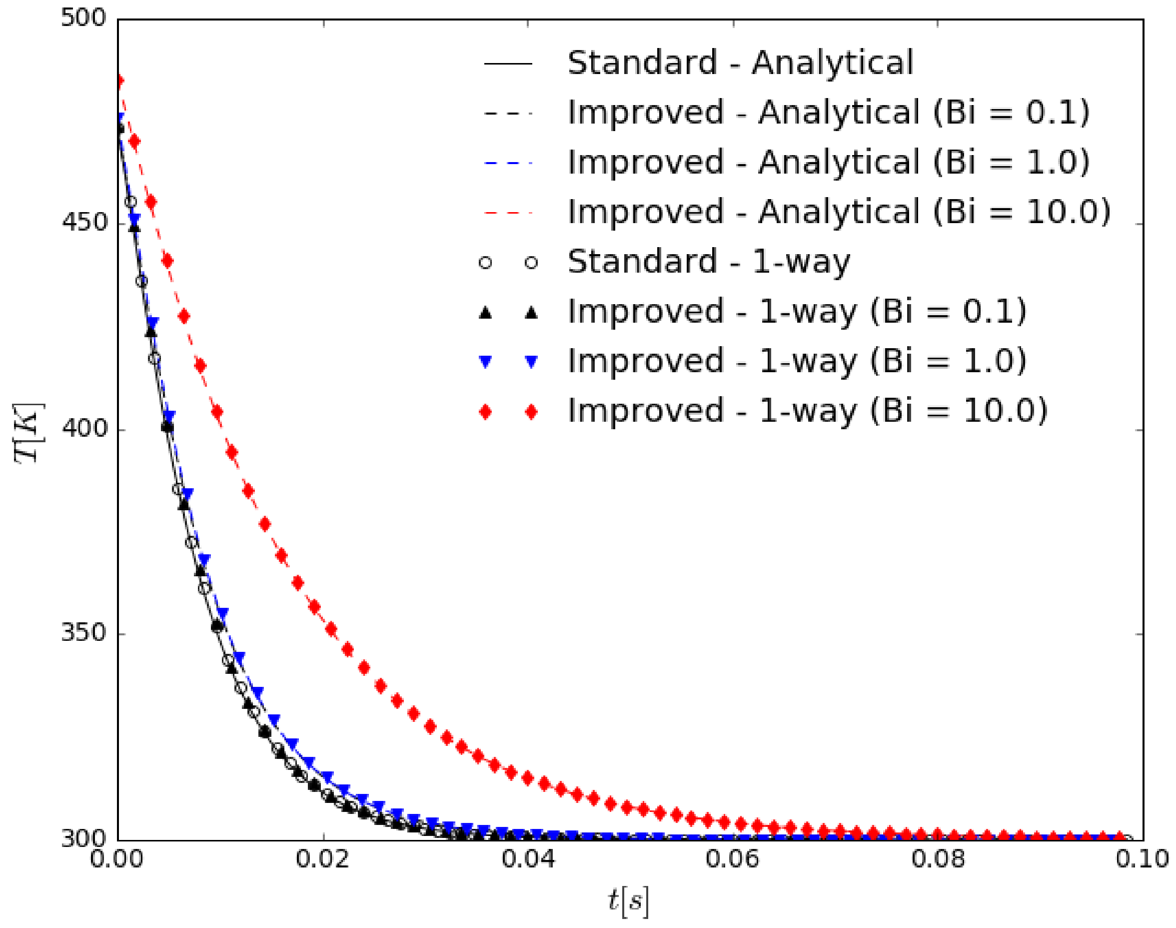
CASE 4 – COOLING PARTICLE WITH IMPROVED FORMULATION

		Value	Unit
Domain	Dimensions	4x8x4	mm
	Mesh size	0.25	mm
Particle	Diameter	0.2	mm
	Density	2500	Kg/m^3
	Heat Capacity	1000	J/kg.K
	Thermal conductivity	**Case dependent**	W/m.K
	Initial temperature	500	K
Water	Viscosity	0.001	Pa.s
	Density	1000	Kg/m^3
	Heat Capacity	5000	J/kg.K
	Thermal conductivity	0.5	W/m.K
	Temperature	300	K



CASE 4 – COOLING PARTICLE WITH IMPROVED FORMULATION

- Standard vs. improved formulation
- Thermal conductivity modified in order to have different Biot numbers
  - Bi =0. 1, 1.0 and 10.0



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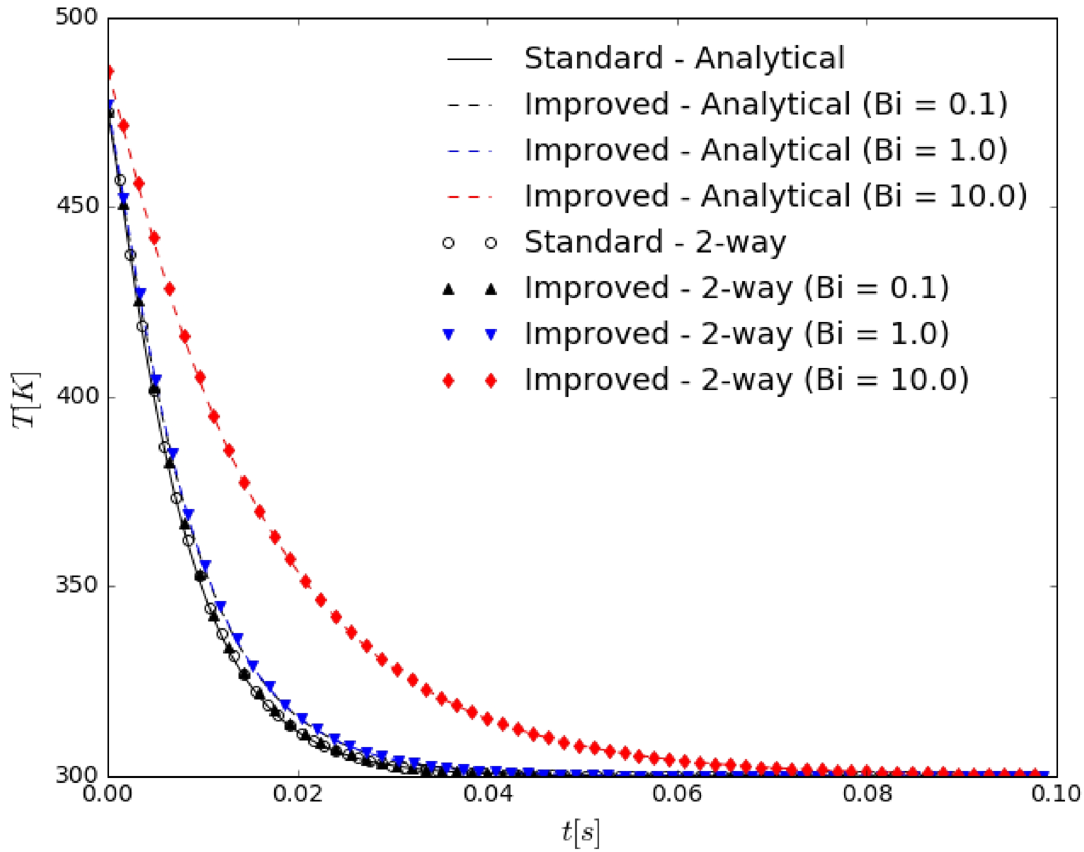
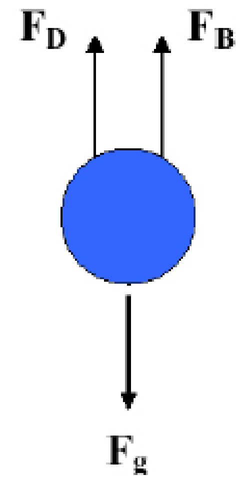


CASE 5 – FALLING PARTICLE WITH HEAT SOURCE



- Cooling particle with volumetric heat source in water

$$m_p \frac{dv_z}{dt} = m_p \left(\rho_p - \rho_f\right) V_p g_z - \frac{1}{2} \rho_f C_D A v_{z_r}^2$$

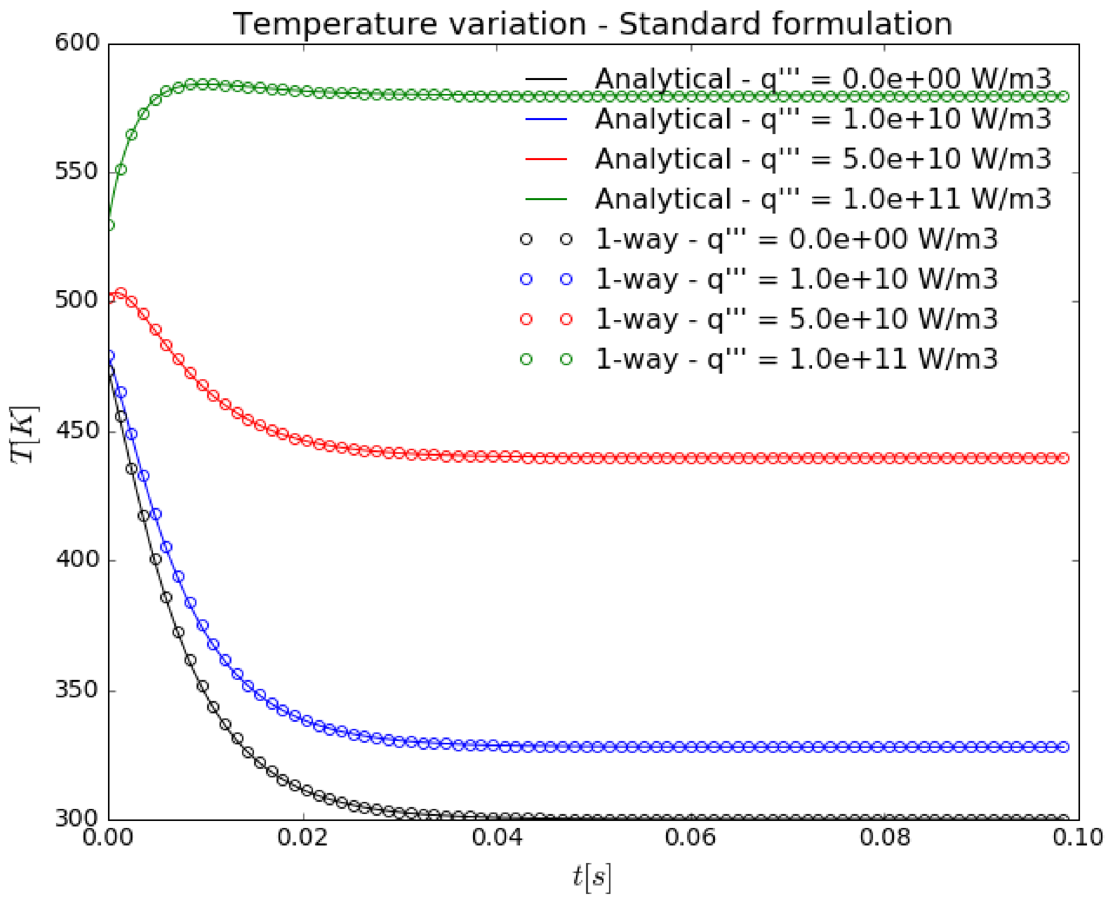
- Schiller & Naumann drag correlation
- Ranz & Marshal correlation for Nusselt number

- Temperature variation as function of heat exchange with water

$$m_p c_p \frac{\partial T_{av}(t)}{\partial t} = A_p h \left(T_m(t) - T_p(R,t)\right) - A_p q'' + V_p q'''$$

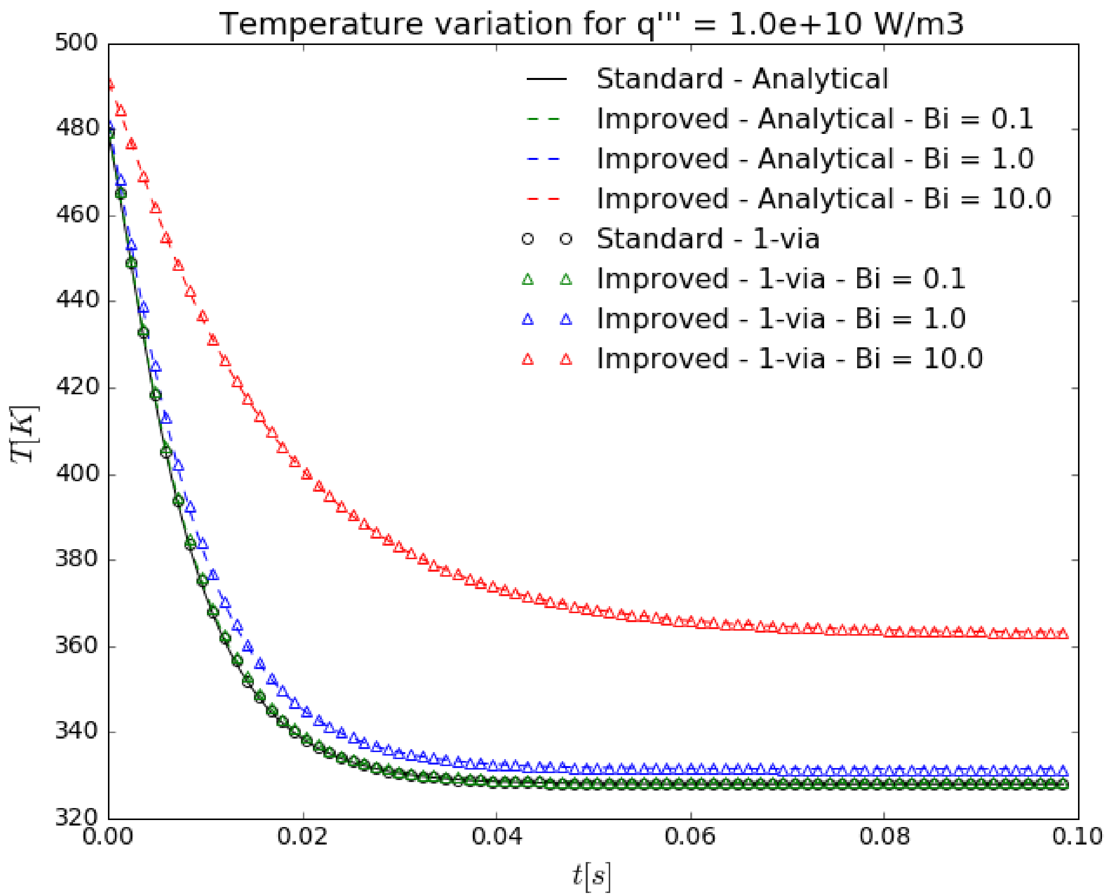
CASE 5 – FALLING PARTICLE WITH HEAT SOURCE

- Standard formulation
- Three different heat source values



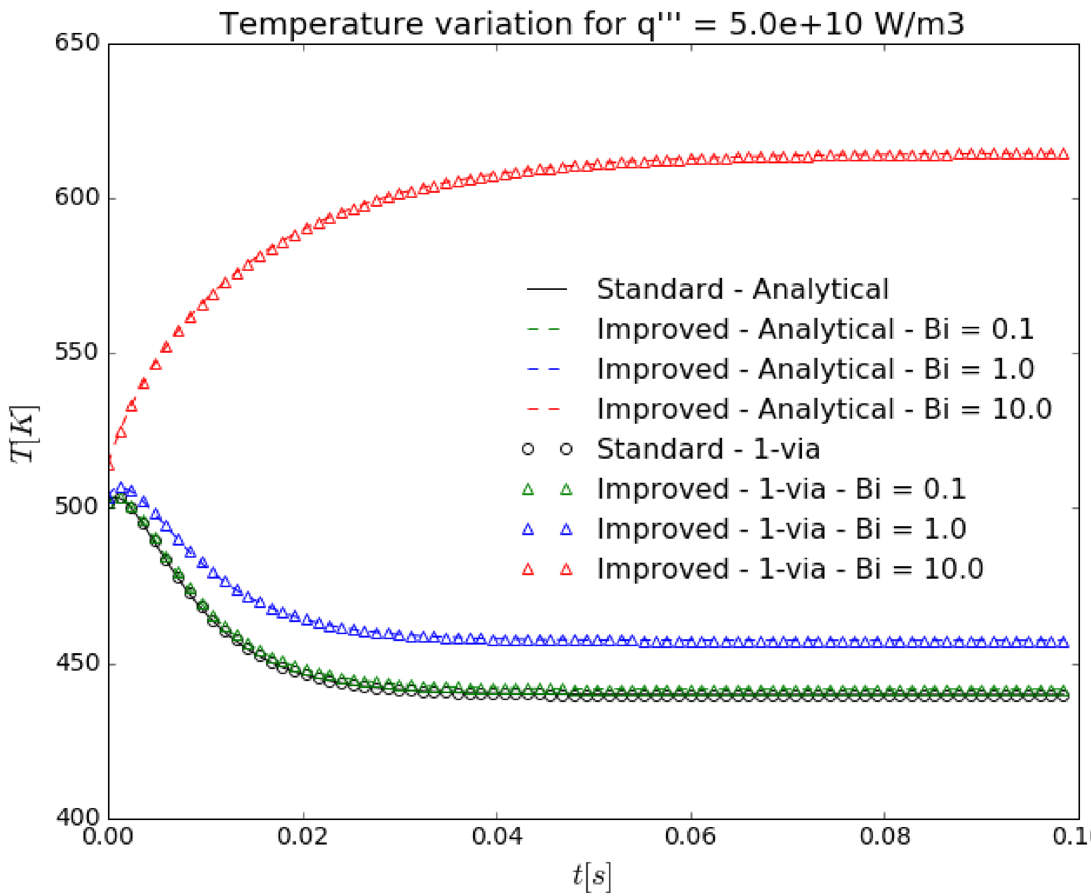
CASE 5 – FALLING PARTICLE WITH HEAT SOURCE

- Standard x improved formulation
- Thermal conductivity modified in order to have different Biot numbers
  - Bi =0. 1, 1.0 and 10.0



CASE 5 – FALLING PARTICLE WITH HEAT SOURCE

- Standard x improved formulation
- Thermal conductivity modified in order to have different Biot numbers
  - Bi =0. 1, 1.0 and 10.0



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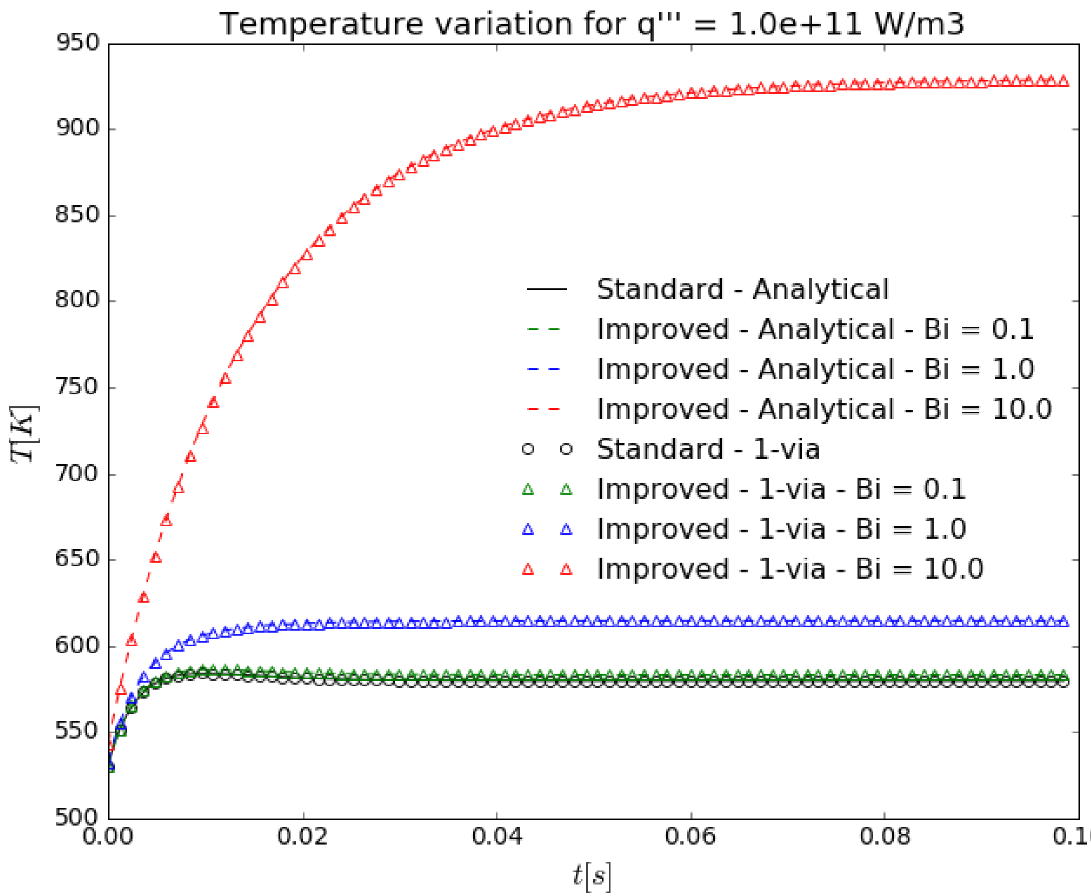


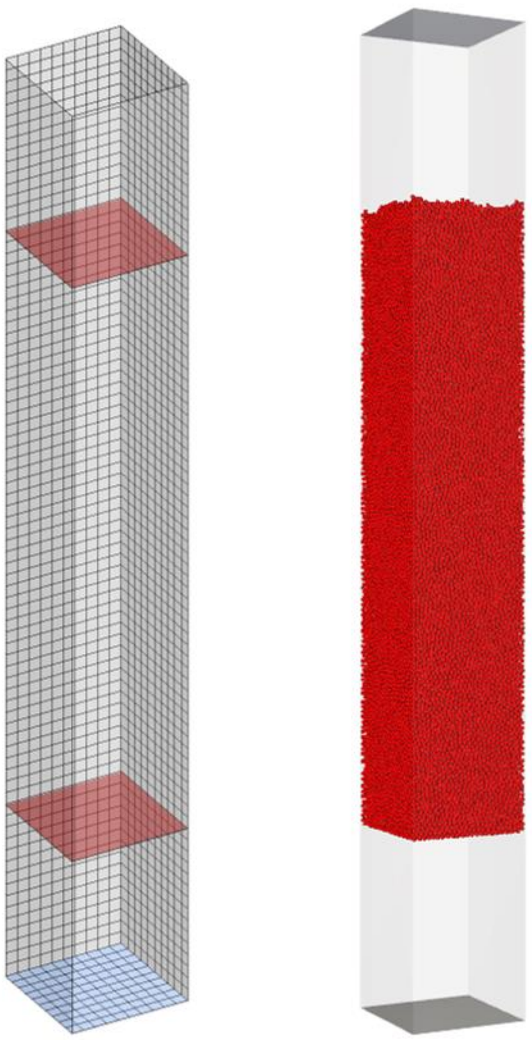
CASE 6 – WATER FLOWING THROUGH FIXED BED

- Water flowing through fixed bed of particles
- Pressure drop comparison against Ergun correlation

$$\frac{\Delta p}{\Delta y} = 150\frac{(1-\epsilon)^2 \mu U}{\epsilon^3 d_p^2} + 1,75\frac{(1-\epsilon)\rho_f U^2}{d_p}$$

- Fluid velocity as function of void fraction

$$u = \frac{U}{\epsilon}$$



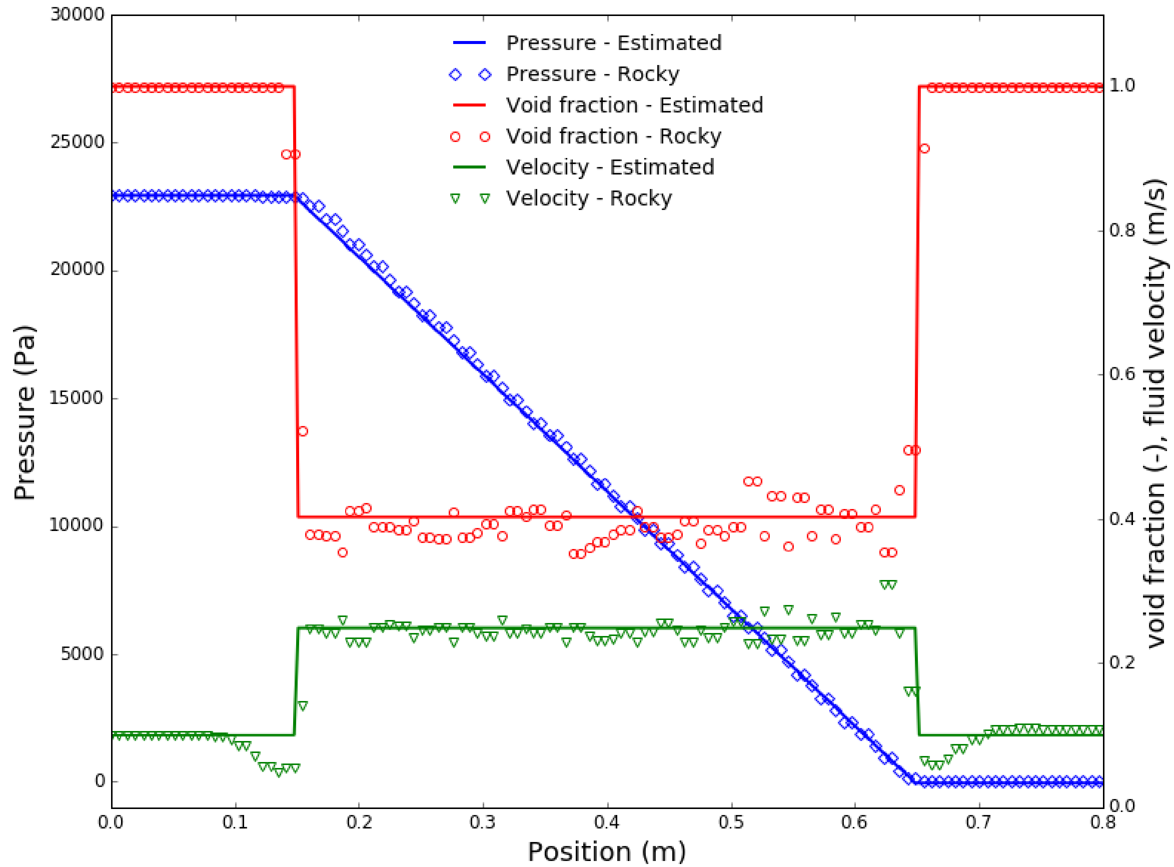
CASE 6 – WATER FLOWING THROUGH FIXED BED

- Huilin & Gidaspow drag corrleation

		Value	Unit
Domain	Dimensions	10x10x80	cm
	Mesh size	10	mm
Particle	Diameter	3.95	mm
	Number of particles	92798	-
	Bed height	0.5	m
	Density	500	Kg/m^3
Water	Viscosity	0.001	Pa.s
	Density	1000	Kg/m^3

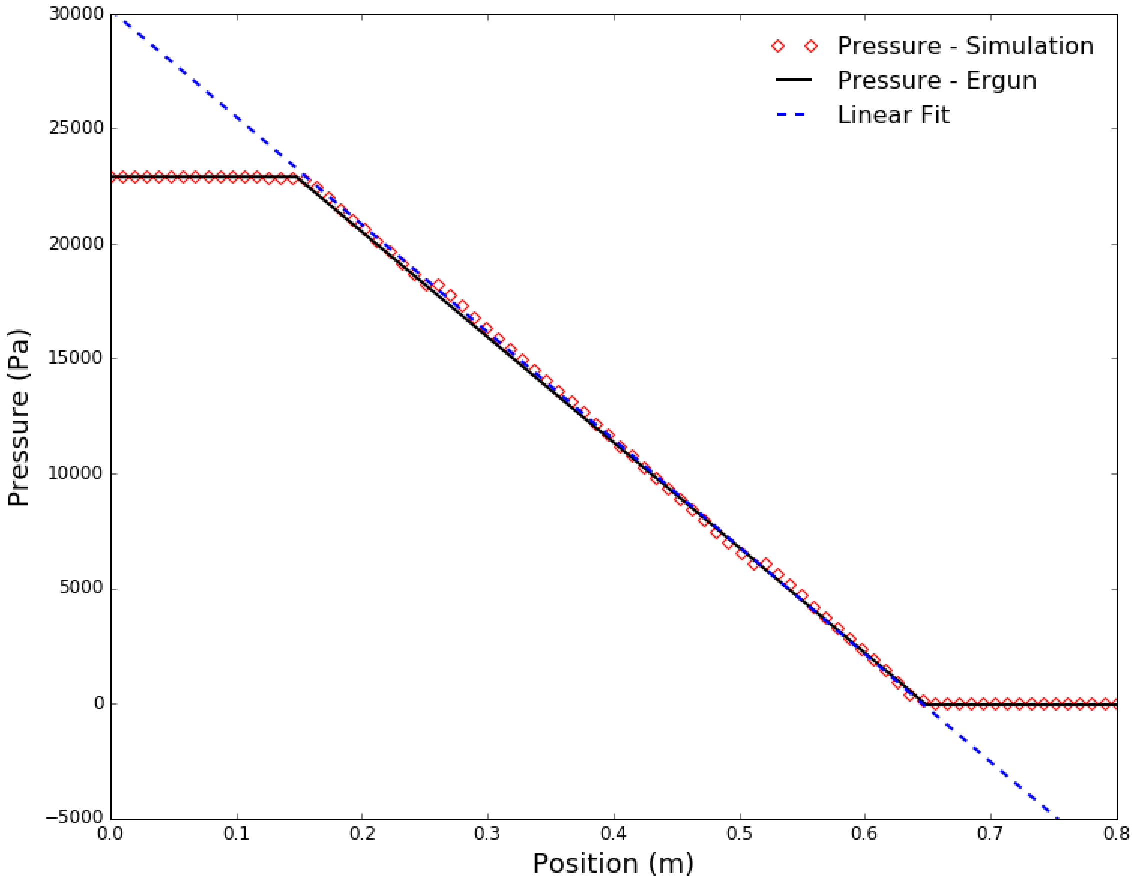
CASE 6 – WATER FLOWING THROUGH FIXED BED

- Velocity and position



CASE 6 – WATER FLOWING THROUGH FIXED BED

- Pressure drop in the bed is 46728 Pa/m
- Ergun's correlation estimative is 45836.77 Pa/m
- Error is 1.94 %



CASE 7 – FLUIDIZED BED

- NETL small scale tests widely used to improve the reliability of computational modeling of multiphase flows by validating with accurate and well defined experimental data

- 3 x 9 x 48 in bubbling fluidized bed
- Geldart D uniform sized particles

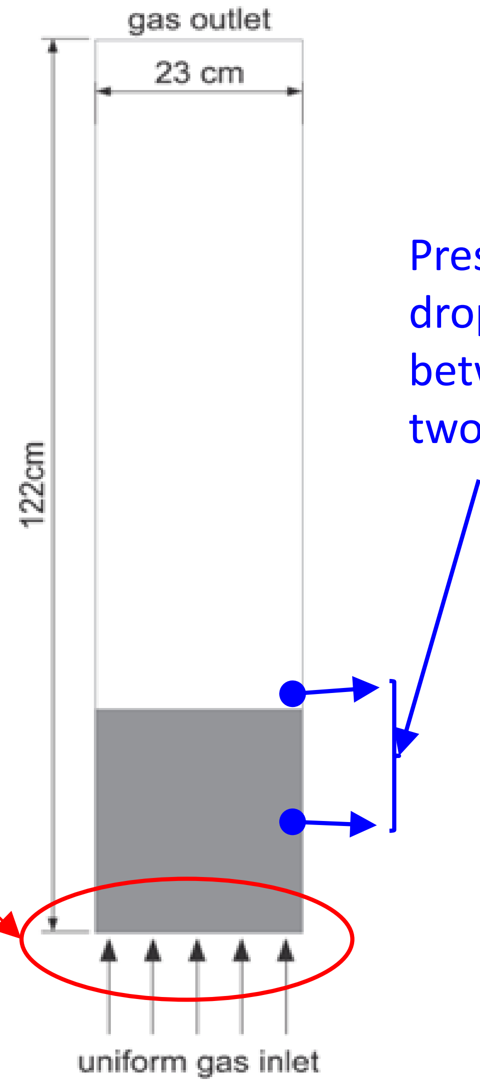
- **2-way coupling test using dense drag law**

(a) SSCP-I test facility and (b) Experimental facility showing pressure intakes

CASE 7 – FLUIDIZED BED

Column with rectangular cross-section

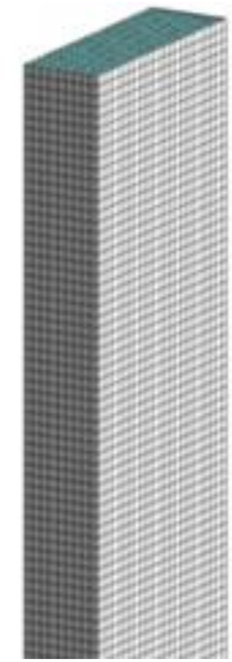
Gas distributor not included



Pressure drop between two intakes

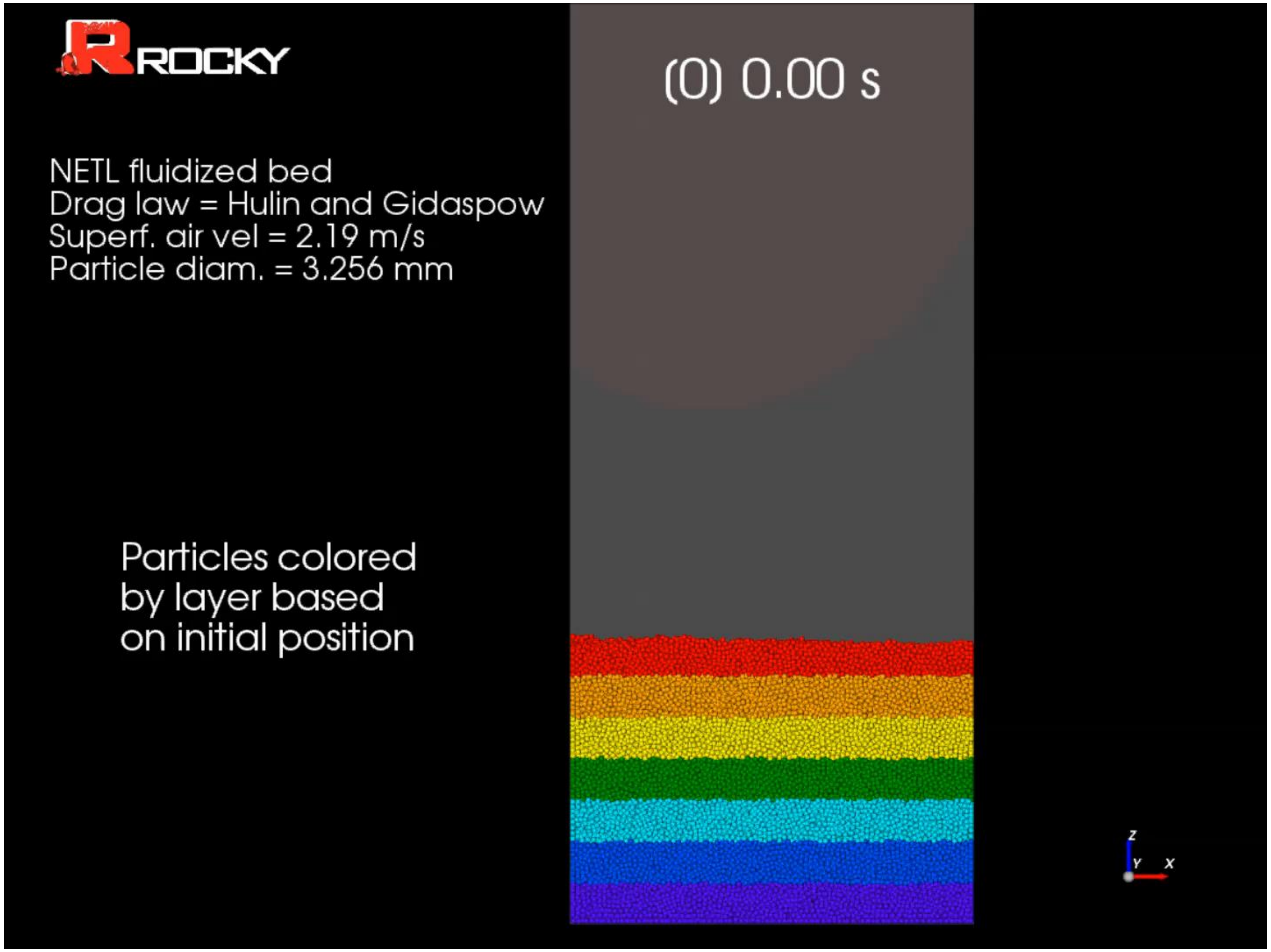
Uniform grid
23808 cells

Cell volume = 50 * particle volume



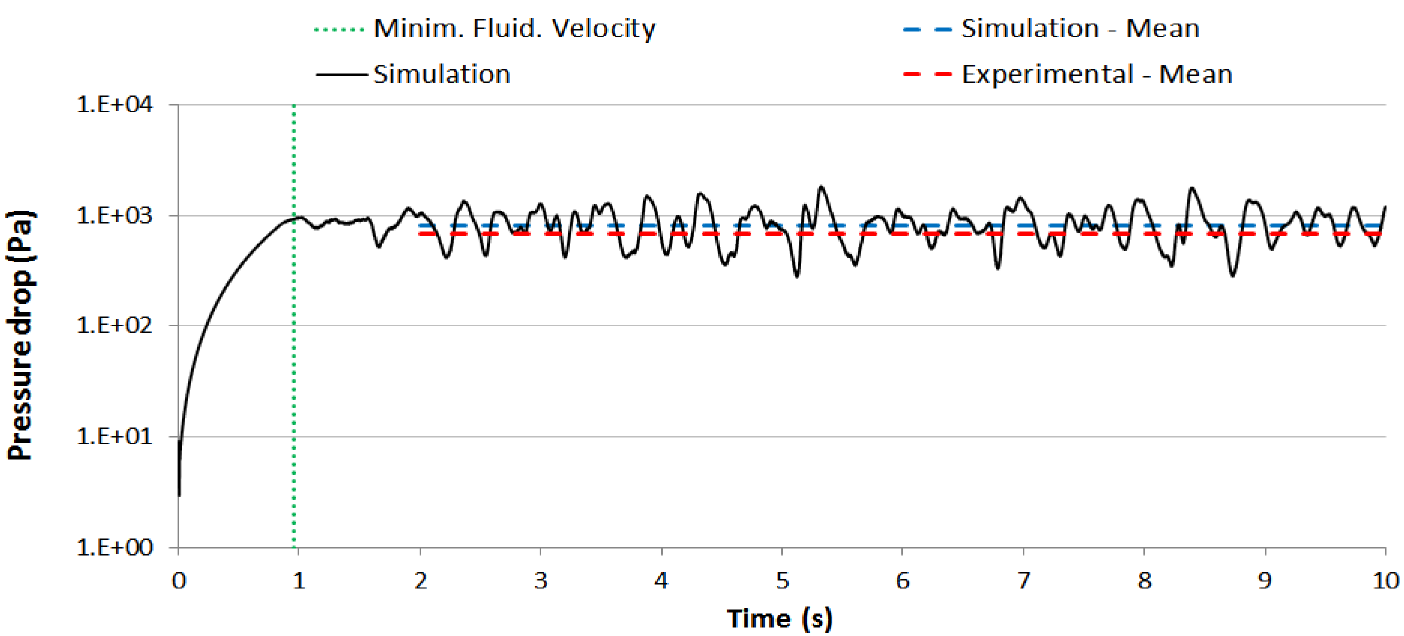
Case	Inlet velocity [m/s]
Small velocity	2.19
Medium velocity	3.28
High velocity	4.38

CASE 7 – PARTICLES BEHAVIOUR



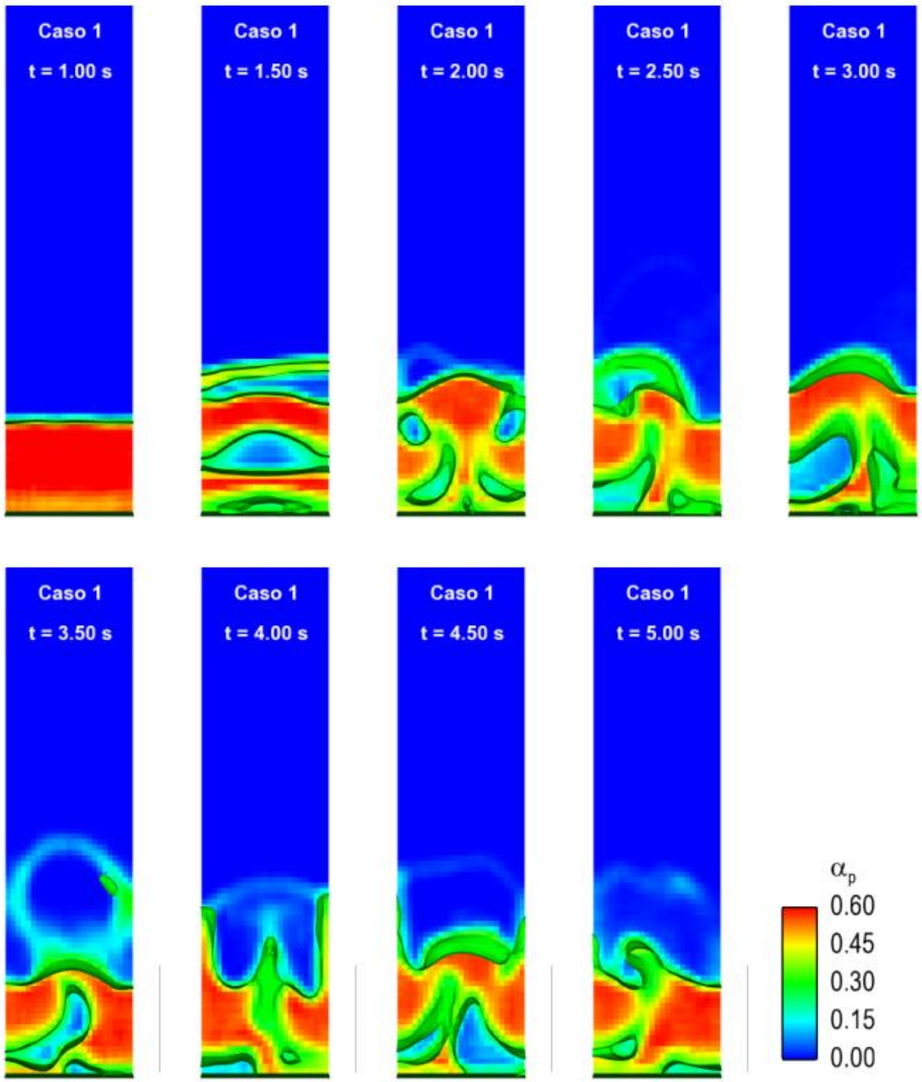
CASE 7 - PRESSURE DROP

- Experimental and simulation minimum fluidization velocities coincide well.
- Good agreement between experimental and simulation pressure drop results after fluidization.



Small velocity case - Evolution of pressure drop between the two pressure intake locations

CASE 7 – BUBBLE/BED DYNAMICS



- Isosurfaces of αp =0.3

- Bubbles formation since Umf, as expected for a Geldart D bed

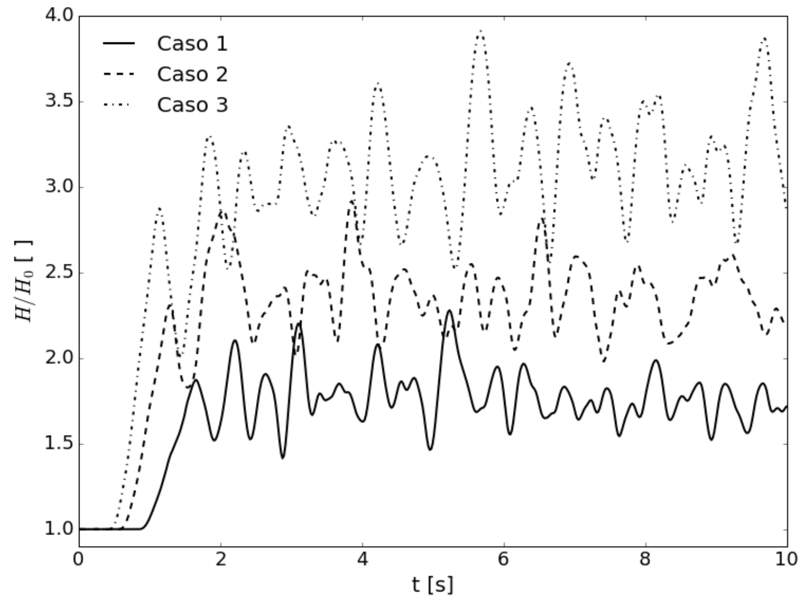
- ↑ gas velocity
- ↑ bubble volume
- ↑ bed height
- ↓ interface definition

CASE 7 – BUBBLE/BED DYNAMICS

$$\langle z_p \rangle = \frac{\sum_k^{N_c} \alpha_{p,k} \; z_{p,k}}{\sum_k^{N_c} \alpha_{p,k}}$$

- Reflects the characteristic fluctuation of bubbling fluidized beds

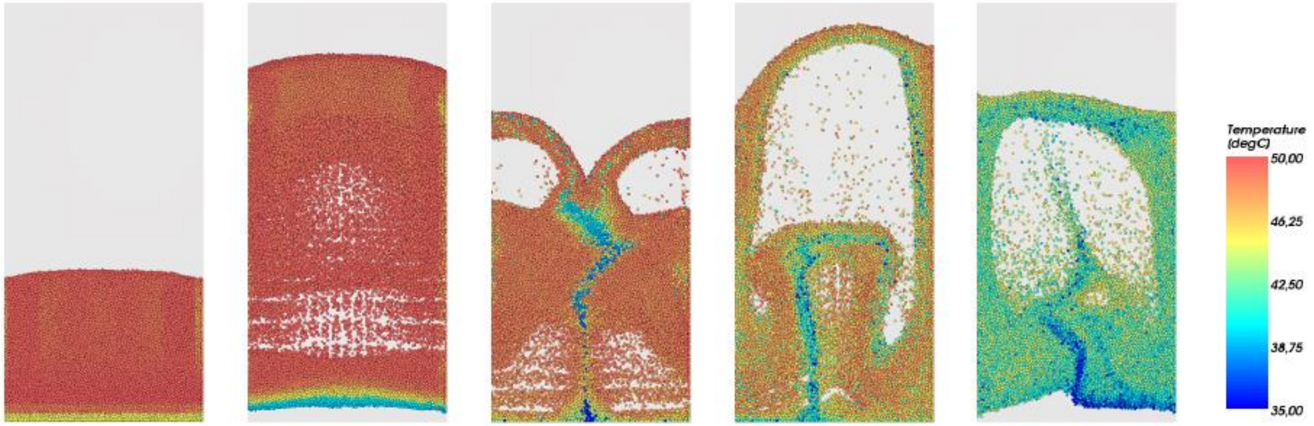
- ↑ gas velocity
- ↑ bed height
- ↑ fluctuations
- Agreement with published results



Time evolution of bed average heights (divided by the initial bed height) for each of the cases

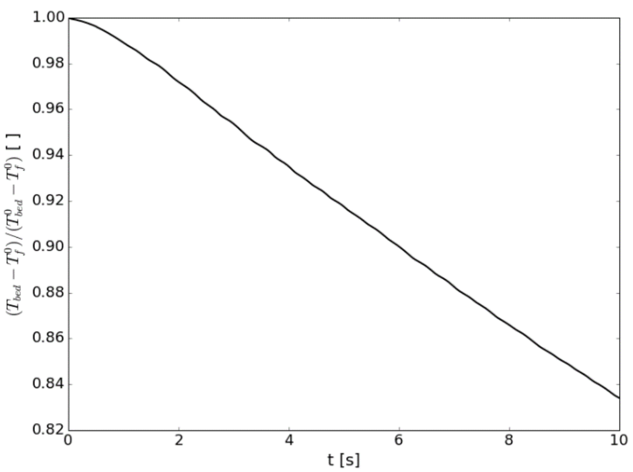
CASE 7 – TEMPERATURE

- Before fluidization, particles at initial position (a)
- First layers have lower T due to heat transfer with cooler gas (b)



(a) 1s (b) 2 s (c) 3 s (d) 5 s (e) 10 s

- After fluidization, particles at the bottom with lower temperatures go upper (c)
- New particles get in contact with cooler gas (d)
- Intimate mixing and agitation result in uniform temperature throughout the bed (e)



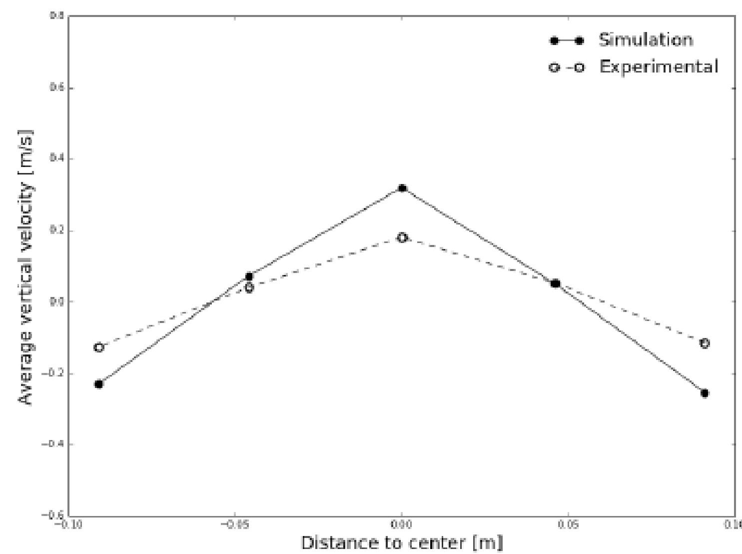
CASE 7 – TEMPERATURE

- Dual recirculation pattern was observed.
- Same pattern reported in literature.

- Average velocity of the particles in 5 different regions of the bed (according to NETL report)

- Positive vertical velocity in the central region where the bubbles carry particles upward

- Negative values near the walls, where the particles return to fill the empty region.



FUTURE DEVELOPMENTS

- PARTICLE SCALE-DOWN MODEL
  - Parcel concept
  - Particle bigger than mesh cell