DEVELOPMENT OF A TWO-FLUID DRAG LAW FOR CLUSTERED PARTICLES USING DIRECT NUMERICAL SIMULATION AND VALIDATION THROUGH EXPERIMENTS

HBCU/MI AWARD DE-FE0007260 REVIEW MEETING
PROGRAM MANAGER: STEVEN SEACHMAN

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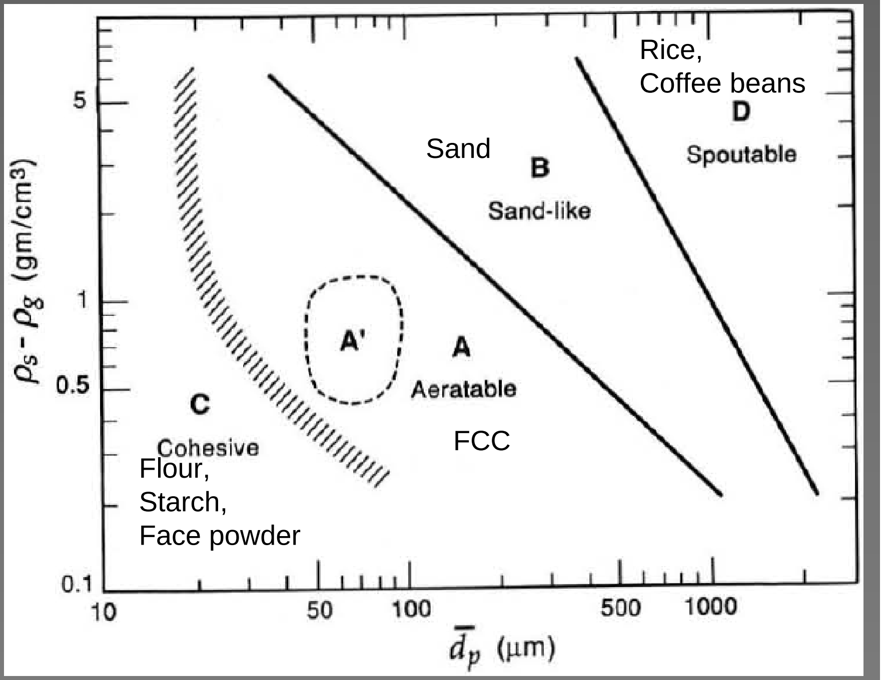
Technical Background

- Particle-resolved direct numerical simulation (DNS) of flow past fixed particle assemblies[3,4,5] yielded a drag relation that is more accurate than the Ergun and Wen-Yu correlations.
- These drag laws are applicable to suspensions where particles do not form clusters, and they have been useful in modeling the hydrodynamics of fluidized beds for Geldart B and D particles[6].

❑ CFD simulation of fluidized beds with Geldart A particles remains a challenge because they fail to reproduce the pressure drop and bed expansion that are observed in experiments[7,8].

- ➢ Formation of particle clusters significantly reduces the drag force.
- ➢ The drag force is overestimated by standard drag laws.



(3) Hill et al., J. of Fluid Mechanics, vol. 448, pp. 243-278, 2001.
(4) Beetstra et al., AIChEJ, vol. 53, pp. 489, 2007.
(5) Tenneti et al., IJMF, 37, 1072-1092, 2011.
(6) van der Hoef et al., Ann. Rev.of Fluid Mech., vol. 40, pp. 47-70, 2008.
(7) Wang et al. Chemical Eng. Sci., vol. 64, no. 3, pp. 622-625, 2009.
(8) Wang, Ind. Eng. Res., vol. 48, no. 12, pp. 5567-5577, 2009.

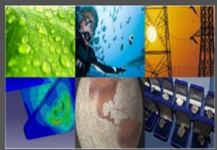
Technical Background

- The current research includes utilization of a combination of numerical and experimental approaches to provide detailed data necessary for validation and optimization purposes.
  - Experimental evaluation of particle clusters will be investigated using high speed imaging.
  - The drag law applicable to particle clustering in fluidized beds will be developed using direct numerical simulations.
  - Finally the developed drag law will be implemented in the MFIX software and the results will be validated against experimental data.

Significance of the results of the work

- Supports the vision of the NETL 2006 Workshop on Multiphase Flow Research[9]:
  - "*To ensure that by 2015 multiphase science based computer simulations play a significant role in the design, operation, and troubleshooting of multiphase flow devices in fossil fuel processing plants*."
- Will develop missing critical constitutive relations to increase the fidelity of CFD models.
- Accurate drag law will result in improved modeling of multiphase flow systems such as fluidized beds and risers.
- Computational advances will be provided to NETL's open-source CFD tool MFIX and validation cases will be provided.

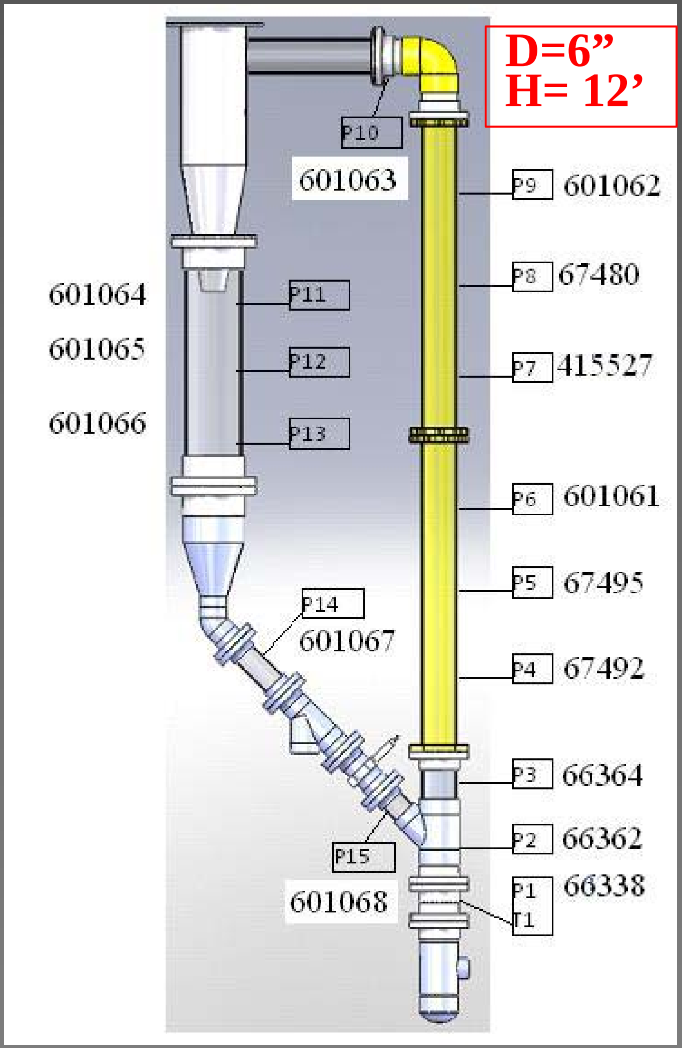
(9) Report on Workshop on Multiphase Flow Research, Morgantown, WV, Ed. M. Syamlal, DOE/NETL-2007/1259, 2006.



Statement of project objectives

- To develop a two-fluid drag-law for clustered particles using direct numerical simulations with experimental validation.
  - Fluidization experiments at the FIU CFB facility:
    - Geldart A type particles to observe clustering of particles,
    - High speed imaging to capture the instantaneous distribution of particles,
    - Convert the images of particle clusters into particle configurations to be used in the DNS.
  - Conduct DNS simulations at ISU:
    - Use the outcome of the DNS for pressure field, velocities of the gas phase and solid particles to calculate the actual drag force on the system of particles.
  - Develop a new drag correlation in the presence of particle clustering and implement in the MFIX computer code. (ISU and FIU)
    - Integrate the new drag-law with MFIX,
    - Simulate the experimental test cases using MFIX with the new drag correlation,
    - Compare the results against the experimental data for pressure drop in the riser.

FIU-ARC CFB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TWO FLUID MODEL

Gas continuity

$$\frac{\partial}{\partial t}(\epsilon_g \rho_g) + \nabla\cdot(\epsilon_g \rho_g \boldsymbol{v}_g) = \sum_{n=1}^{N_g} R_{gn}$$

Solids continuity

$$\frac{\partial}{\partial t}(\epsilon_s \rho_s) + \nabla\cdot(\epsilon_s \rho_s \boldsymbol{v}_s) = \sum_{n=1}^{N_s} R_{sn}$$

Gas momentum

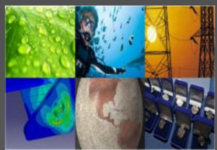
$$\frac{\partial}{\partial t}(\epsilon_g \rho_g \boldsymbol{v}_g) + \nabla\cdot(\epsilon_g \rho_g \boldsymbol{v}_g \boldsymbol{v}_g) = \nabla\cdot\bar{\bar{S}}_g + \epsilon_g \rho_g \boldsymbol{g} - \boldsymbol{I}_{gs}$$

Gas-phase stress

$$\bar{\bar{S}}_g = -\epsilon_g P_g \bar{\bar{I}} + \bar{\bar{\tau}}_g = -\epsilon_g P_g \bar{\bar{I}} + 2\epsilon_g \mu_g \bar{\bar{D}}_g + \epsilon_g \lambda_g tr(\bar{\bar{D}}_g)\bar{\bar{I}}$$

Gas Energy Equation

$$\varepsilon_g \rho_g C_{pg}\left(\frac{\partial T_g}{\partial t} + \vec{v}_g . \nabla T_g\right) = -\nabla . \vec{q}_g - H_{g1} - H_{g2} - \Delta H_{rg} + H_{wall}(T_{wall} - T_g)$$



TWO FLUID MODEL

Solids momentum

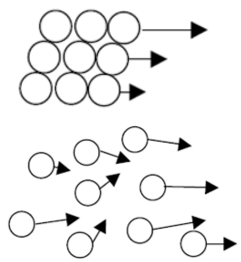
$$\frac{\partial}{\partial t}(\epsilon_s \rho_s \boldsymbol{v}_s) + \nabla\cdot(\epsilon_s \rho_s \boldsymbol{v}_s \boldsymbol{v}_s) = \nabla\cdot\bar{\bar{S}}_s + \epsilon_s \rho_s \boldsymbol{g} - \nabla P_g - F_{gs}(\boldsymbol{v}_s - \boldsymbol{v}_g)$$

Solids−phase stress

$$\bar{\bar{S}}_s = \begin{cases} -P_s^p \bar{\bar{I}} + \bar{\bar{\tau}}_s^p, & \text{if} \quad \epsilon_g \le \epsilon_g^* \\ -P_s^v \bar{\bar{I}} + \bar{\bar{\tau}}_s^v & \text{if} \quad \epsilon_g > \epsilon_g^* \end{cases}$$

$$P_s^p = 10^{25}(\epsilon_s - \epsilon_s^{cp})^{10}$$

$$P_s^v = 2(1+e)\rho_s g_0 \epsilon_s^2 \Theta_s$$

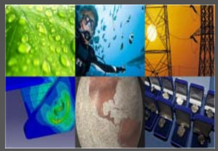


$$\bar{\bar{\tau}}_s^v = 2\mu_s^v \bar{\bar{D}}_s + \lambda_s^v tr(\bar{\bar{D}}_s)\bar{\bar{I}} \qquad \mu_s^v = K_3 \epsilon_s \sqrt{\Theta}_s \qquad \lambda_s^v = K_2 \epsilon_s \sqrt{\Theta}_s$$

$$\bar{\bar{\tau}}_s^p = 2\mu_s^p \bar{\bar{D}}_s \qquad \mu_s^p = P_s^p \sin\phi / 2\sqrt{I_{2D}}$$

Definition of K1, K2, k3, k4 in slide 5

$$I_{2D} = ((D_{s11} - D_{s22})^2 + (D_{s22} - D_{s33})^2 + (D_{s33} - D_{s11})^2)/6 + D_{s12}^2 + D_{s23}^2 + D_{s31}^2$$



TWO FLUID MODEL

Algebraic Equation of the Granular Temperature

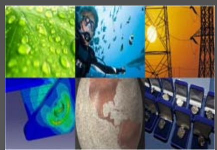
$$\Theta = \left\{ \frac{-K_1 \epsilon_s \mathrm{tr}(\overline{\overline{D}}_s) + \sqrt{K_1^2 \epsilon_s^2 tr^2(\overline{\overline{D}}_s) + 4K_4 \epsilon_s [K_2 tr^2(\overline{\overline{D}}_s) + 2K_3 tr(\overline{\overline{D}}_s^2)]}}{2K_4 \epsilon_s} \right\}^2$$

$$K_{1m} = 2\,(1+e_{mm})\,\rho_m\, g_{0_{mm}} \qquad K_{2m} = 4\, d_{pm}\,\rho_m\,(1+e_{mm})\,\varepsilon_m\, g_{0_{mm}} / (3\sqrt{\pi}) - \frac{2}{3} K_{3m}$$

$$K_{3m} = \frac{d_{pm}\,\rho_m}{2} \left\{ \frac{\sqrt{\pi}}{3(3-e_{mm})} [0.5(3\,e_{mm}+1) + 0.4(1+e_{mm})(3\,e_{mm}-1)\,\varepsilon_m\, g_{0_{mm}}] + \frac{8\,\varepsilon_m\, g_{0_{mm}}(1+e_{mm})}{5\sqrt{\pi}} \right\}$$

$$K_{4m} = \frac{12\left(1-e_{mm}^{\ 2}\right)\ \rho_{sm}\ g0_{mm}}{d_{pm}\sqrt{\pi}} \qquad g0_{lm} = \frac{1}{\varepsilon_g} + \frac{3\,d_{pl}\,d_{pm}}{\varepsilon_g^{\ 2}\left(d_{pl}+d_{pm}\right)} \sum_{\lambda=1}^{M} \frac{\varepsilon_{s\lambda}}{d_{p\lambda}}$$

Radial distribution function



TWO FLUID MODEL

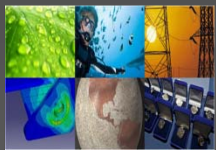
Transport Equation of the Granular Temperature

$$\frac{3}{2}\left[\frac{\partial}{\partial t}\left(\rho_s\alpha_s\theta_s\right)+\nabla\cdot\left(\rho_s\alpha_s\vec{v}_s\theta_s\right)\right]=\left(-p_s\bar{\bar{I}}+\bar{\bar{\tau}}_s\right):\nabla\cdot\left(k_{\theta_s}\nabla\theta_s\right)-\gamma_{\theta_s}+\phi_{ls}\;;$$

$$k_{\theta_s}=\frac{150\,\rho_s\,d_s\sqrt{(\theta\pi)}}{384\,(1+e_{ss})\,g0_{,ss}}\left[1+\frac{6}{5}\alpha_s\,g0_{,ss}\,(1+e_{ss})\right]^2+2\rho_s\alpha_s{}^2 d_s(1+e_{ss})g0_{,ss}\sqrt{\frac{\theta_s}{\pi}}$$

$$\gamma_{\theta_m}=\frac{12\left(1-e^2{}_{ss}\right)g0_{,ss}}{d_s\sqrt{\pi}}\rho_s\alpha_s{}^2\theta_s{}^{3/2}\;;$$

$$\phi_{ls}=-3K_{ls}\theta_s$$



TWO FLUID MODEL

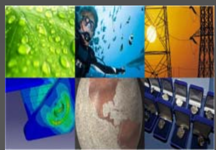
Gas-Solid Drag Force

O'Brien and Syamlal Drag model

$$F_{gs} = \frac{3\epsilon_s \epsilon_g \rho_g}{4V_{rs}^2 d_p} C_{Ds}\left(\frac{Re_s}{V_{rs}}\right)\left|\boldsymbol{v}_s - \boldsymbol{v}_g\right|$$

$$V_{rs} = 0.5\left(A - 0.06 Re_s + \sqrt{(0.06 Re_s)^2 + 0.12 Re_s (2B - A) + A^2}\right.$$

$$A = \epsilon_g^{4.14}, \qquad B = \begin{cases} c\epsilon_g^{1.28} & \text{if} \quad \epsilon_g \le 0.85 \\ \epsilon_g^{d} & \text{if} \quad \epsilon_g > 0.85 \end{cases}$$



Type equation here.Clustering criterion

Cohesive inter-particle van der Waals forces $\mathbf{F}_{ij}^{(c)} = \frac{Ad}{12Z_{ij}^2}\mathbf{n}_{ij}$ [1]

Scaling factor φ used by Ye et al. 2005 [1]

$$\varphi = \frac{|U_{min}|}{K_B\ T} = \frac{A\ d}{12\ Z_0} \cdot \frac{1}{K_B T}$$

dp $\leq$ 100 mm,

nij : Surface normal vector
A : Hamaker constant ~ 10^{-19} J for FCC[2]
d : center to center distance
Z_0 : cut off surface to surface distance clustered consideration
K_B : Boltzmann constant ~ 1
T : granular temperate
d/Z0 ~ 2.5x 10^5 [2]

Clustering criterion

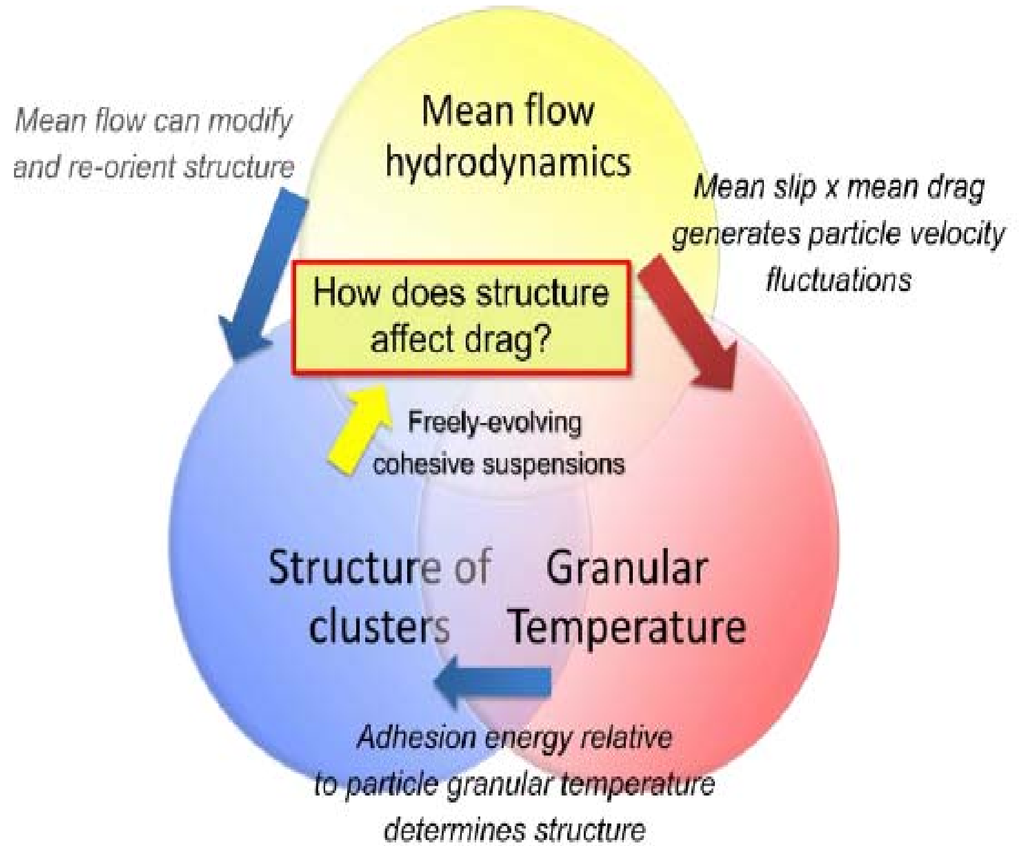
Governing equations for particle motion

$$\frac{d\mathbf{X}^{t}}{dt} = V^{(i)}$$

$$m_{eff}\frac{dV^{(i)}}{dt} + \frac{AR_S}{6r^2}$$

$m_{eff} = m1m2/ (m1+ m2)$
X particle position
V particle velocity
r surface-to-surface distance
A Hamaker constant
R surface effective curvature $=d_p/2$

Interaction of solid and gas mean flow



Clustering criterion

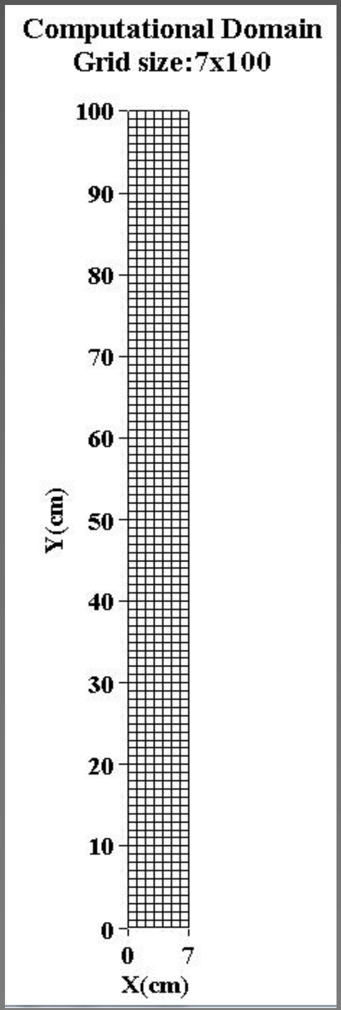
Scaling factor Ha used in this research :

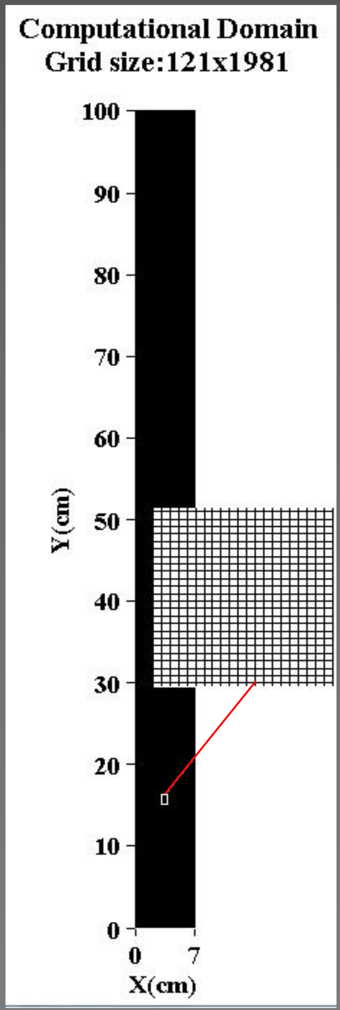
measure of the adhesive potential to the characteristic kinetic energy

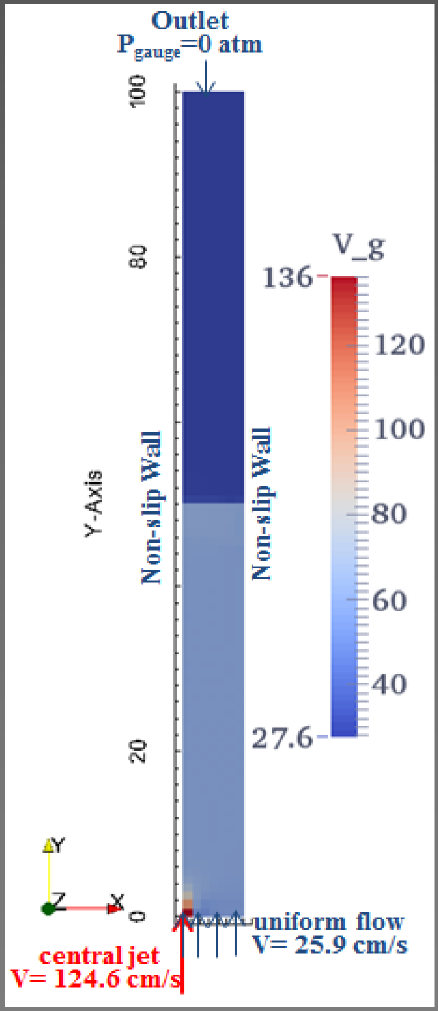
$$\boxed{Ha = \frac{A}{\rho \pi d_p^2 d_0 T}}$$

A : Hamaker constant ~ 10^{-19} J for FCC[2]
d_p : Particle diameter
Z0 : cut off surface to surface distance clustered consideration
d_0 : cut off surface to surface distance for clustered consideration
T : granular temperature
dp/d0~ 10^4

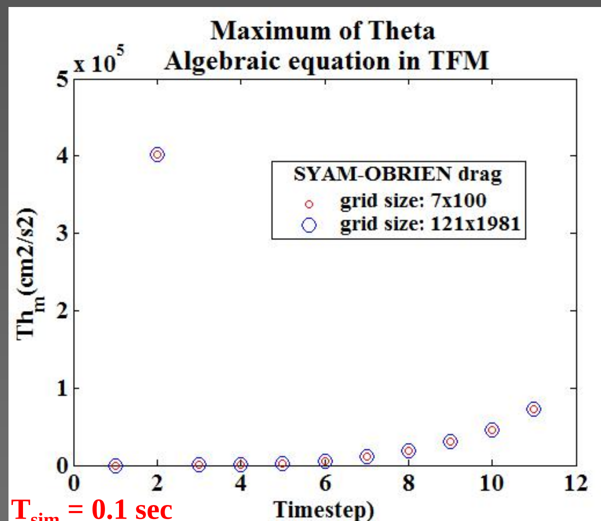
Computational Domain

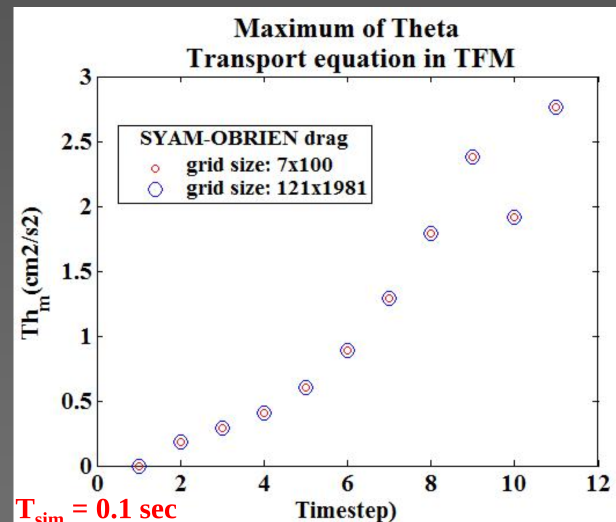


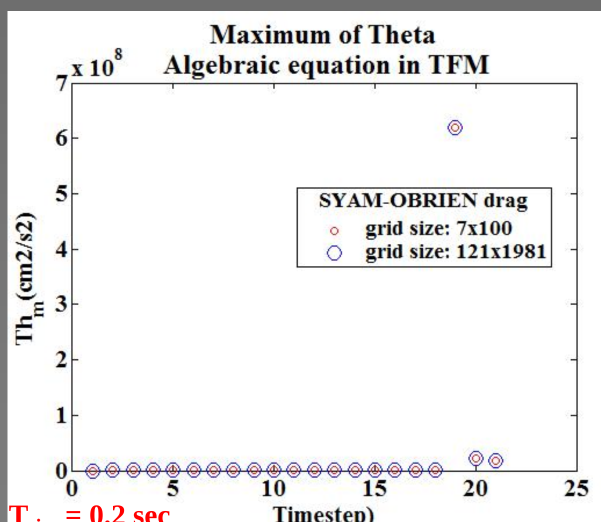


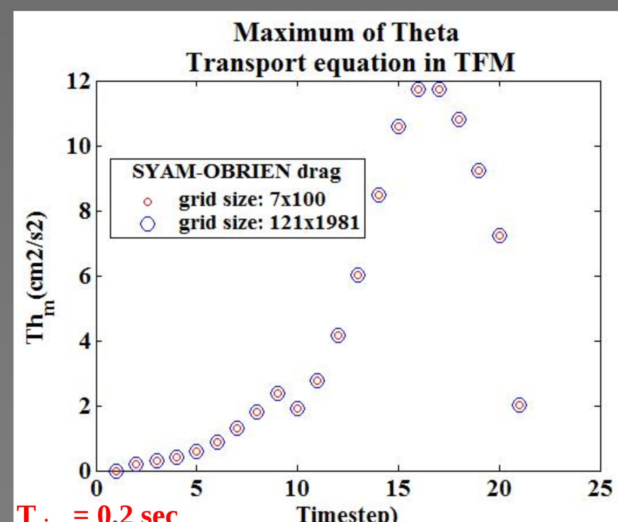


Granular temperature : Algebraic versus Transport Equation

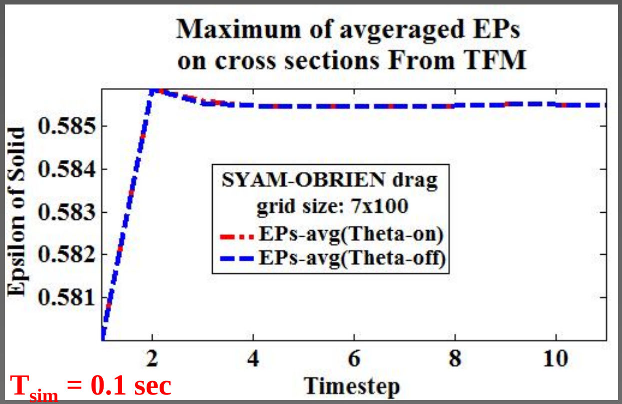


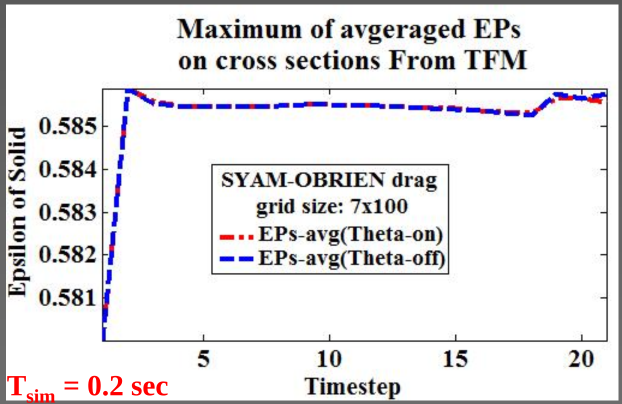


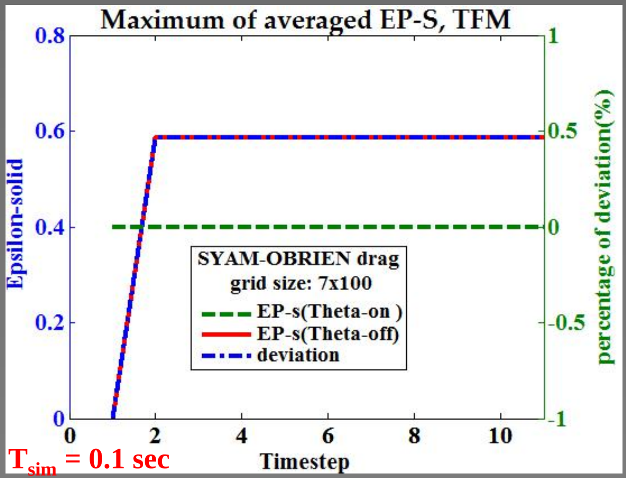


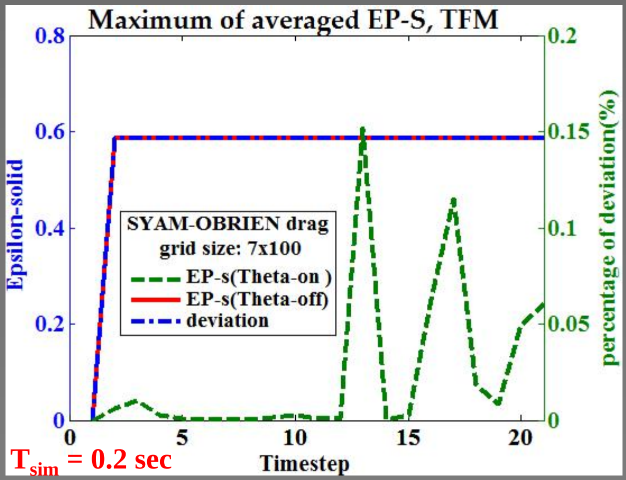


Variation in simulation results : Algebraic versus Transport Equations for Θ

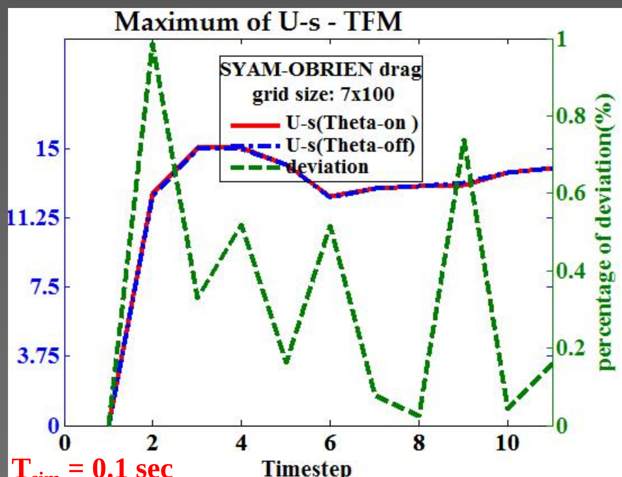


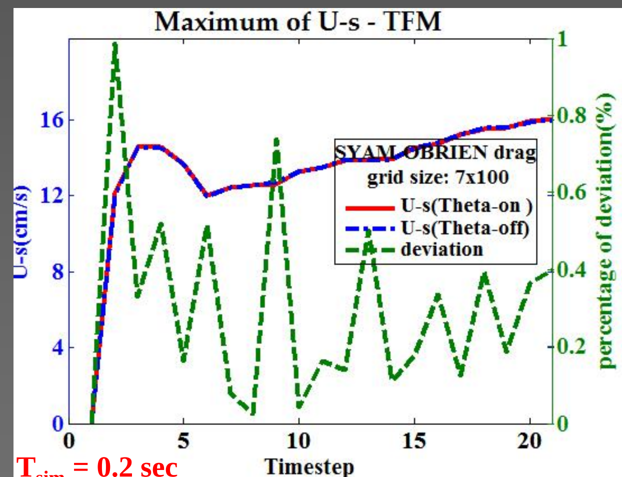


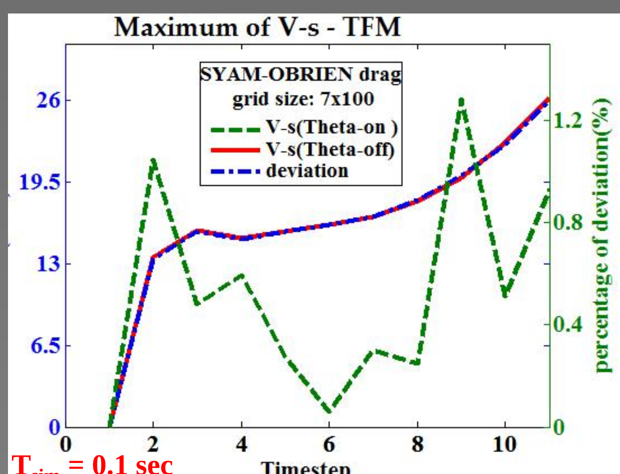


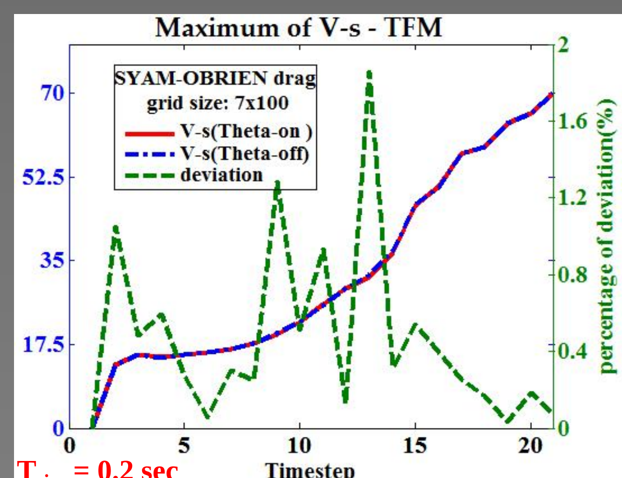


Variation in simulation results : Algebraic versus Transport Equations for Θ



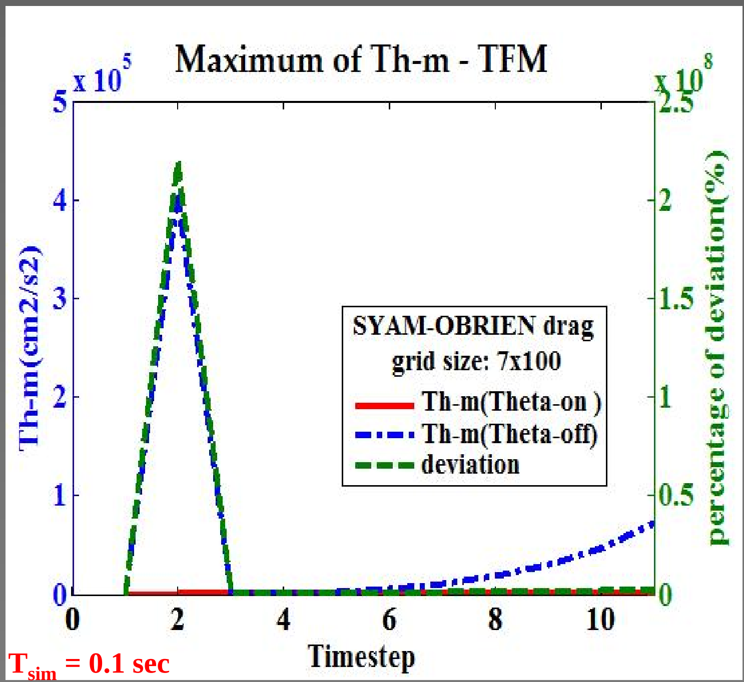


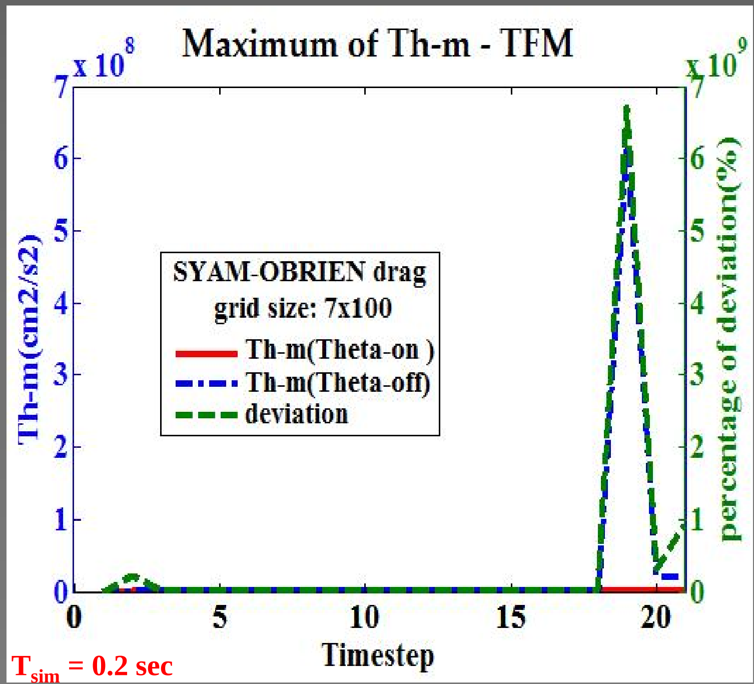


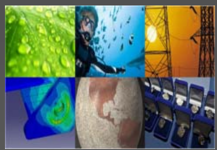


Variation in simulation results : Algebraic versus Transport Equations for Θ

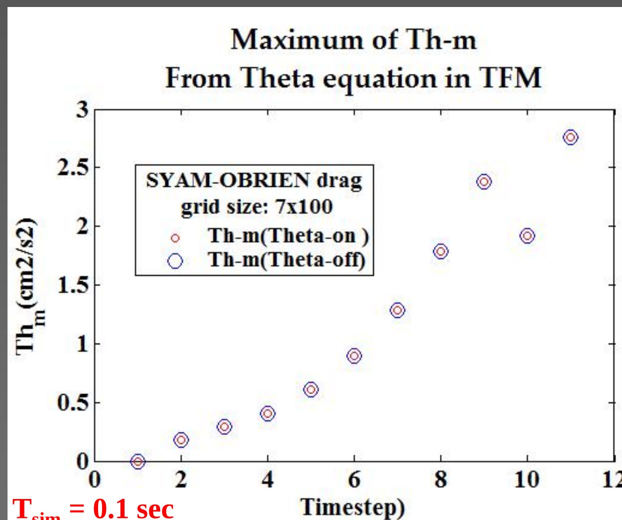
Variance in theta increases as the simulation progresses

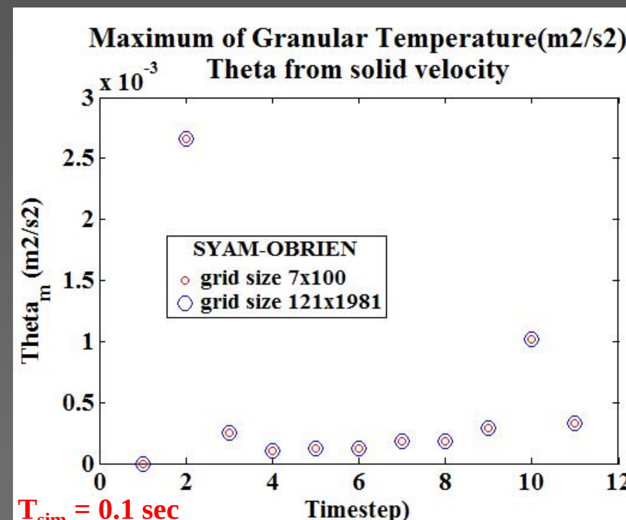


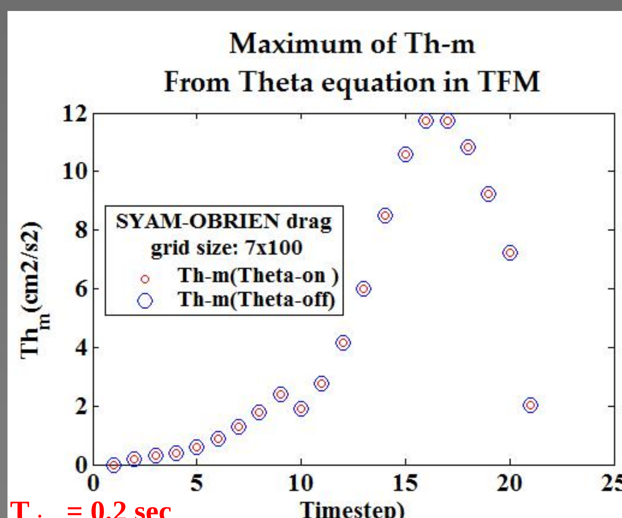


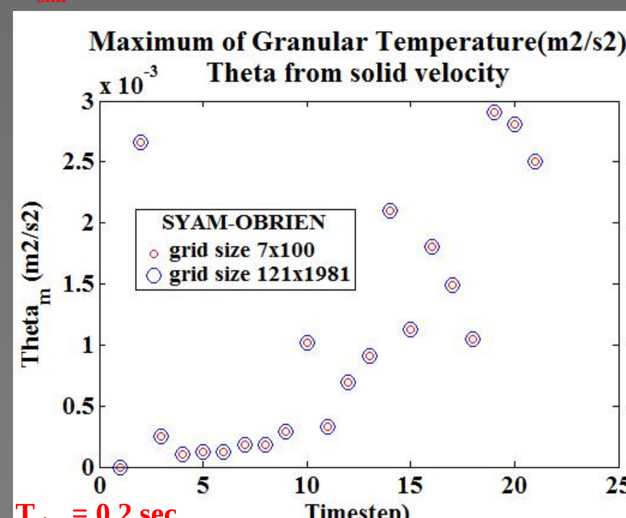


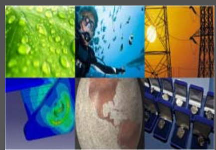
Variation in simulation results : versus Transport Equations for Θ



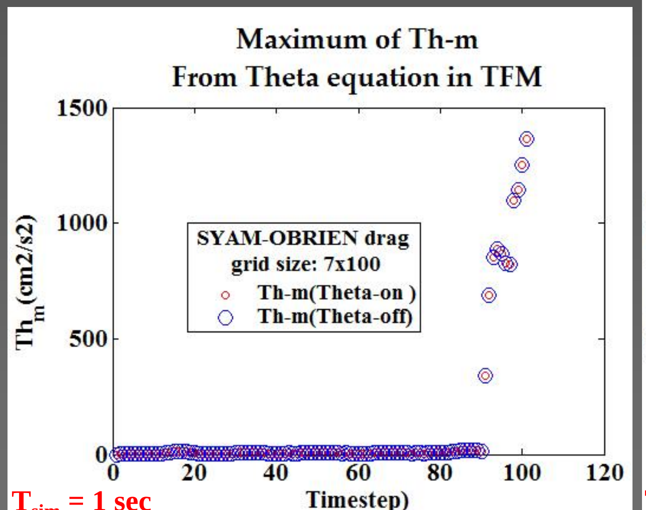


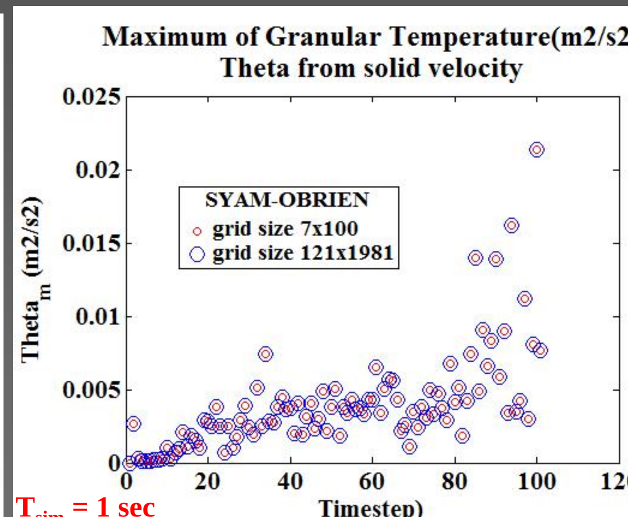


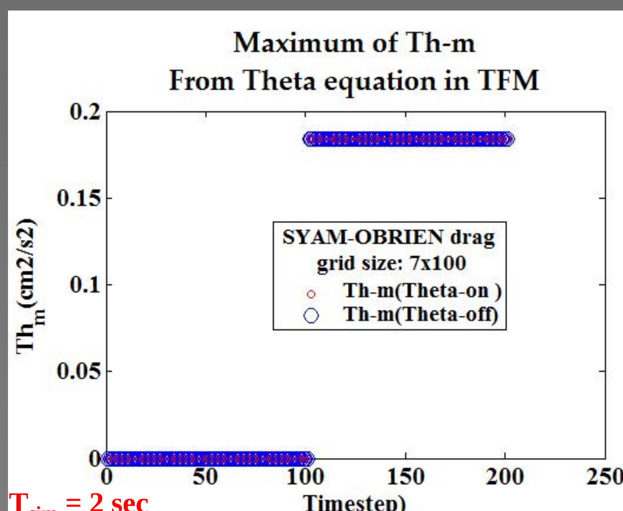


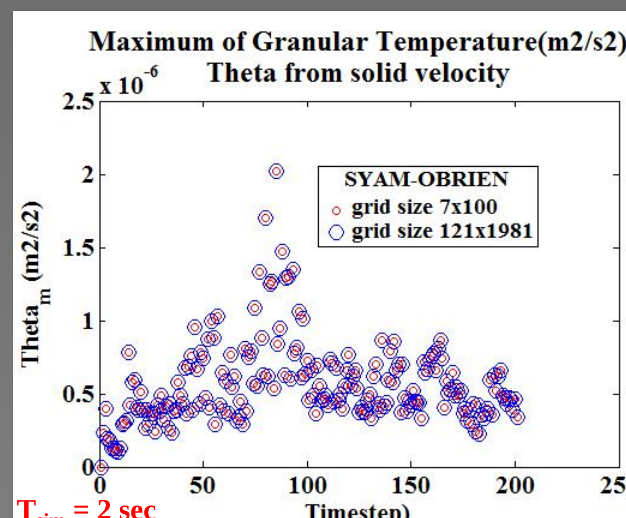


Calculation of Theta from solids velocities





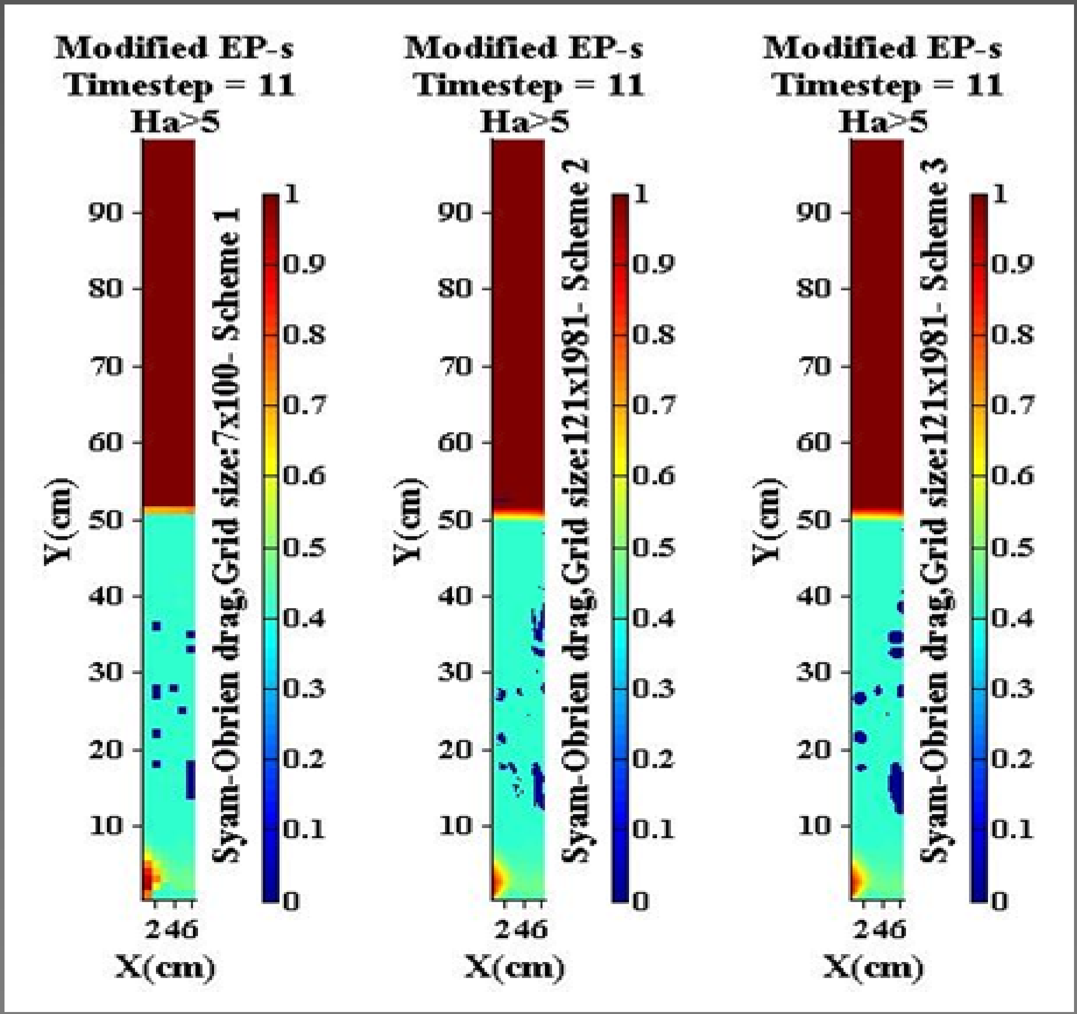




Calculation and implementation of the Ha parameter

$$Ha = \frac{A}{\rho \pi d_p^2 d_0 T}$$

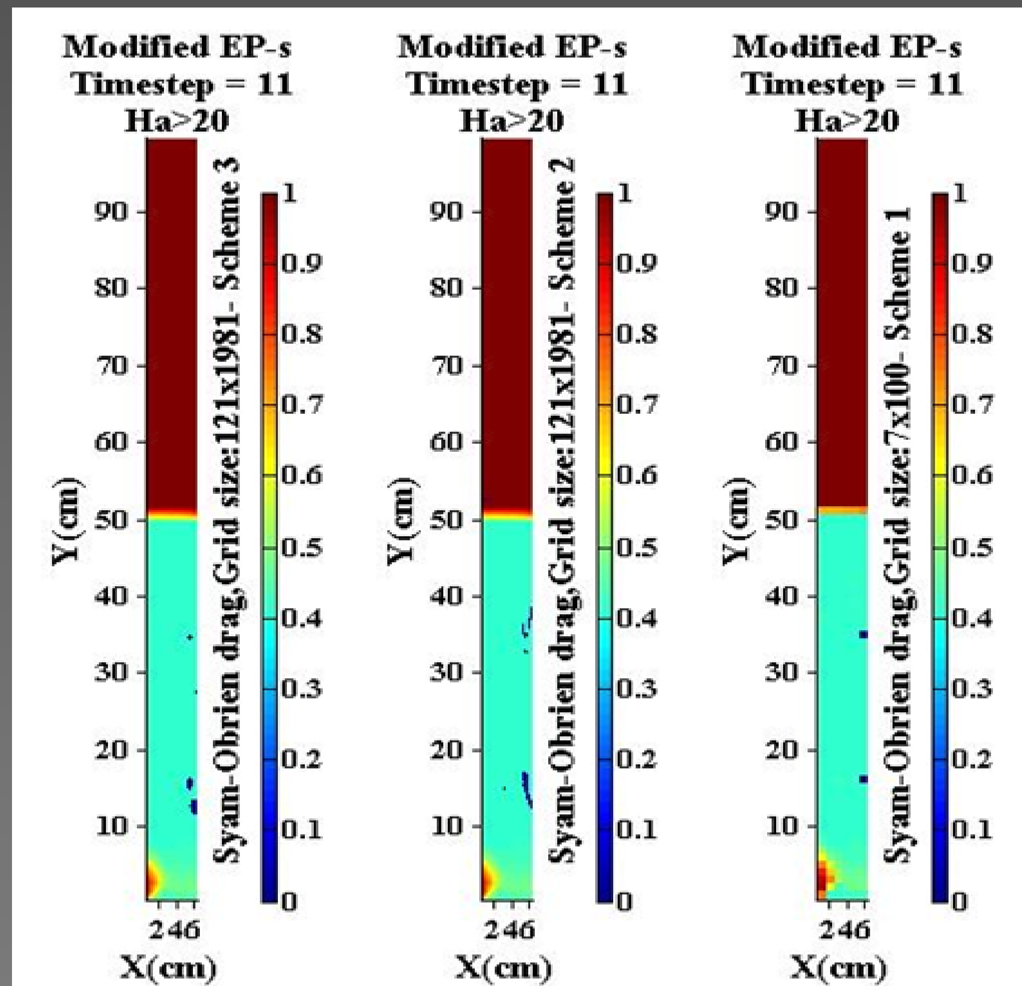
Modification to gas volume fraction due to implementation of the Ha parameter, thresholding Ha>5



Calculation and implementation of the Ha parameter

$$Ha = \frac{A}{\rho \pi d_p^2 d_0 T}$$

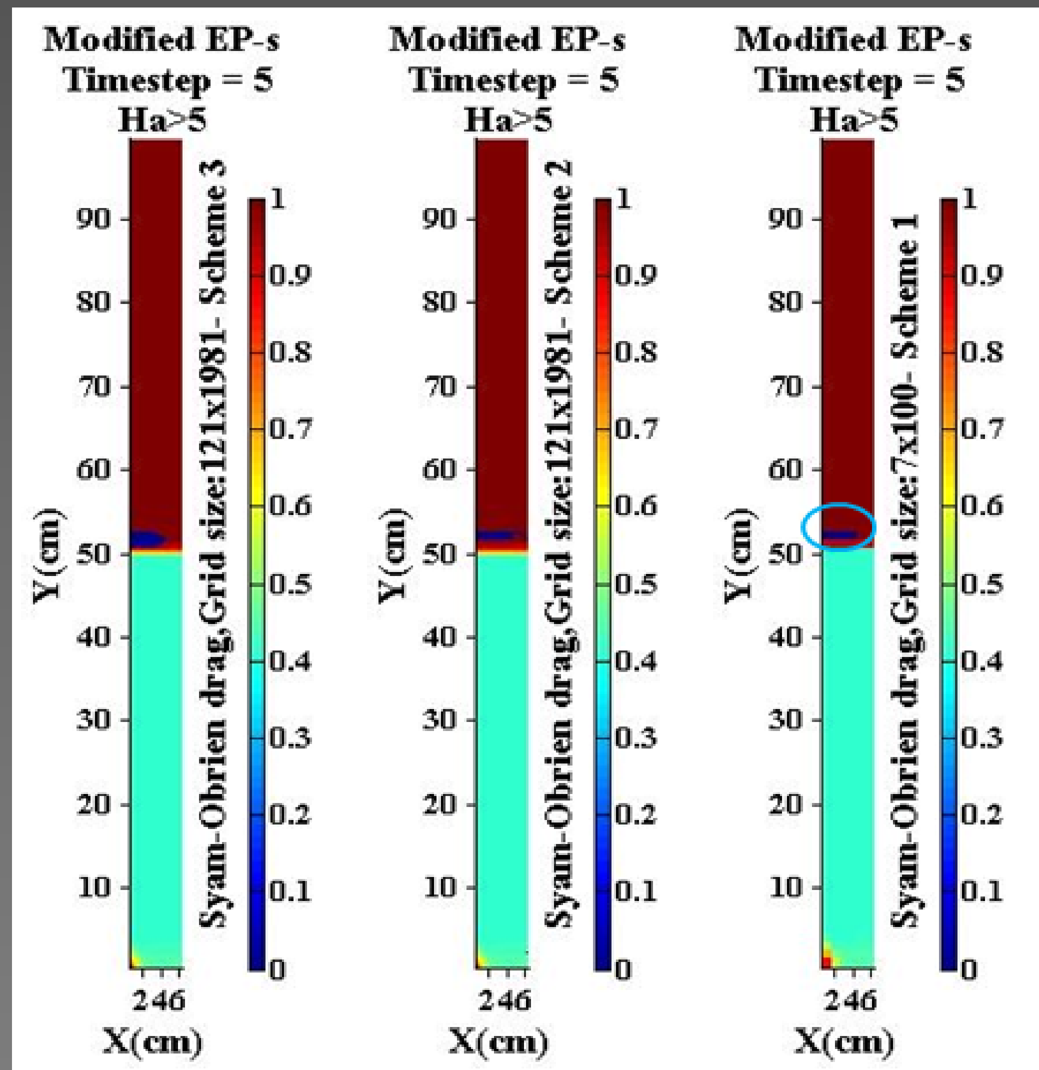
Modification to gas volume fraction due to implementation of the Ha parameter, Thresholding Ha>20



Calculation and implementation of the Ha parameter

$$Ha = \frac{A}{\rho \pi d_p^2 d_0 T}$$

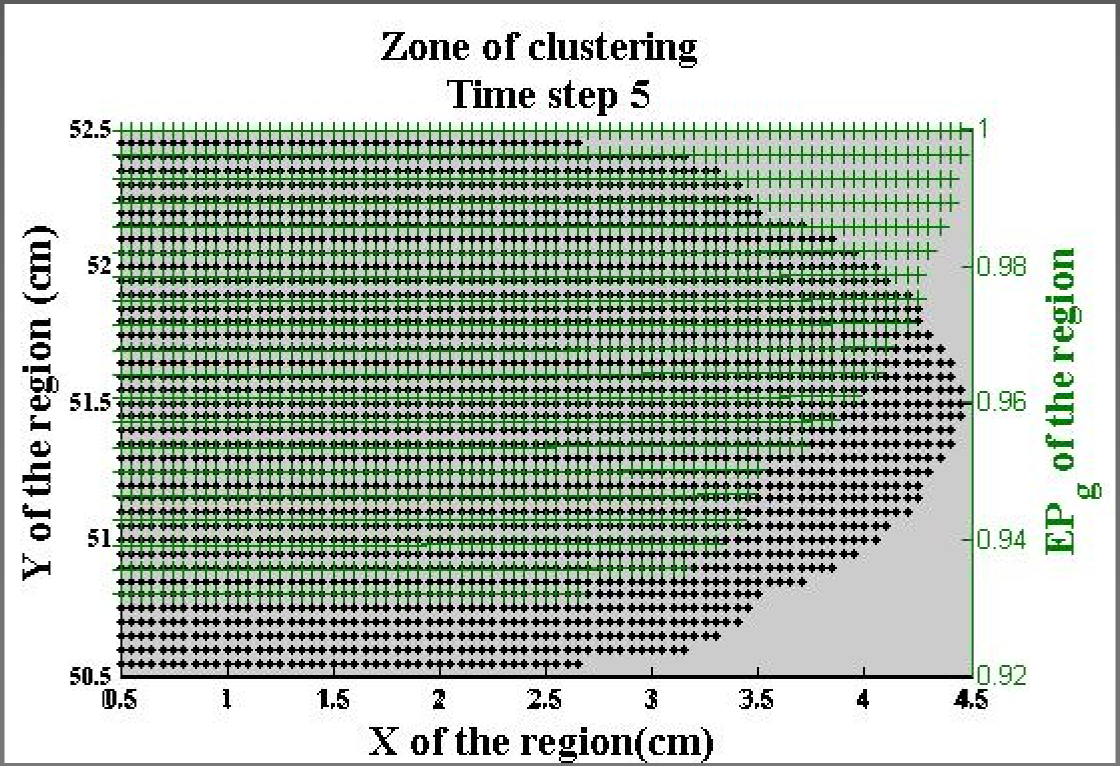
Non-physical results
Generation of clusters in suspicious regions



Performance evaluation of the Ha criteria

Non-physical results
Generation of clusters in suspicious regions

EP-g > 0.94 in a candidate region for clustering formation

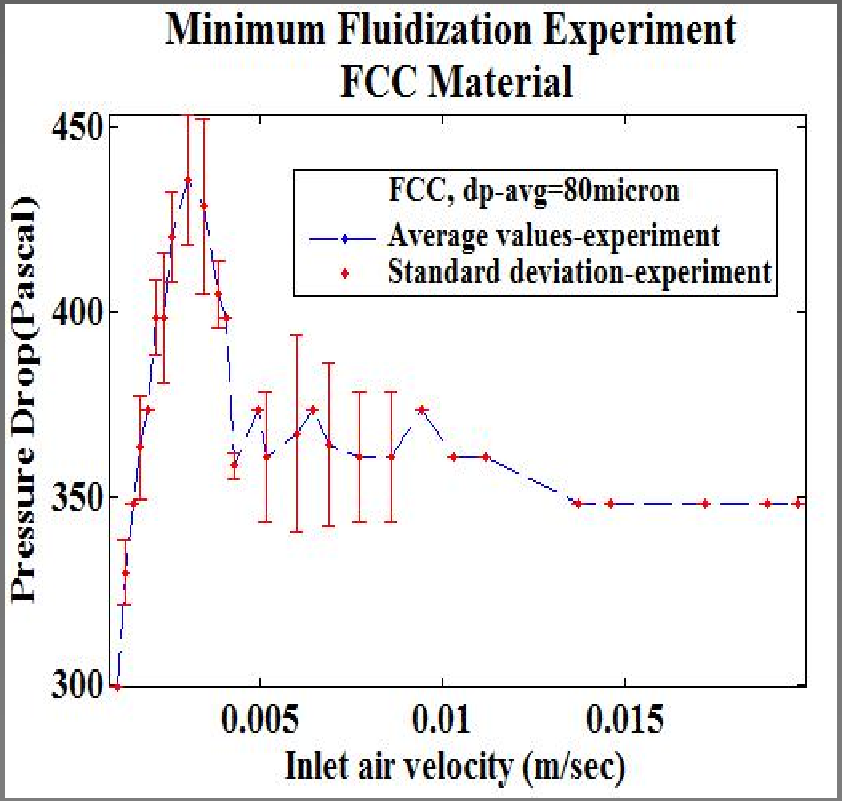


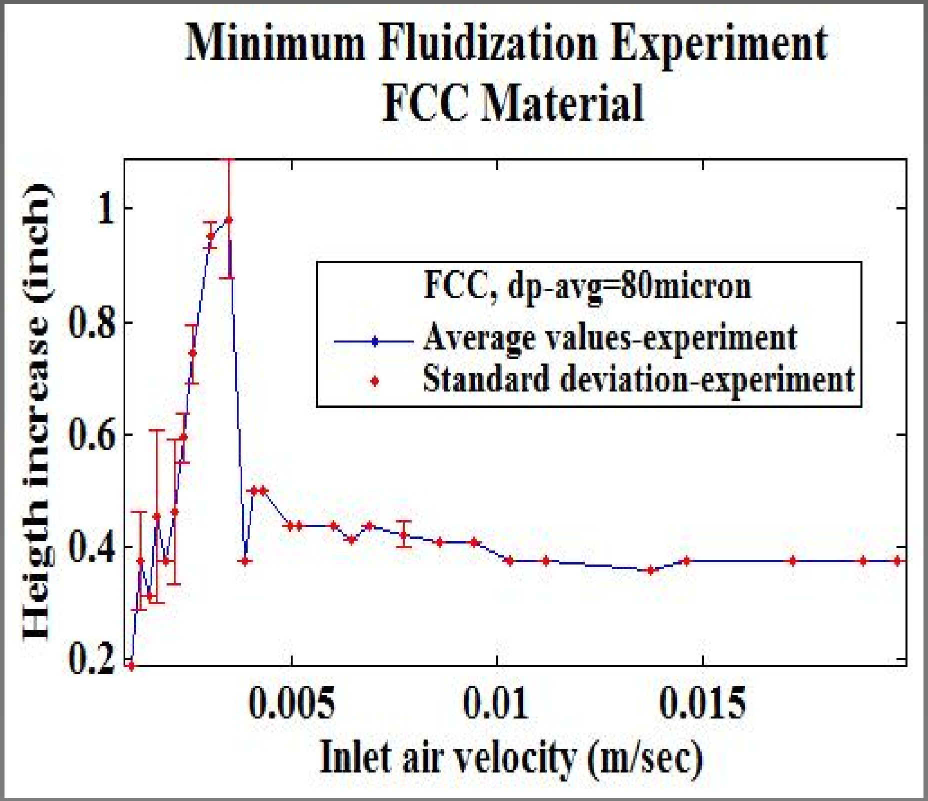
Experimental work
Minimum fluidization experiment

Measuring pressure drop and bed height expansion in a Minimum Fluidization experiment for the FCC material

Experimental work
Minimum Fluidization Experiment

Measuring pressure drop and bed height expansion in a minimum fluidization experiment for the FCC material

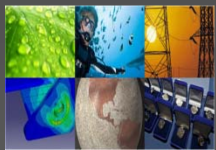




Conclusions

Effect of different methods for estimating granular temperature on important field variables :

- Divergence of results obtained from the algebraic equation of the granular temperature
- Increase of the error with increase of simulation time



Conclusions

- Significant differences between results of the granular temperature from the solution of the algebraic equation and solution of the coupled systems of transport equations

- Significant differences between results of the granular temperature in sequential times steps and solution of the coupled systems of transport equations

Conclusions

- The Ha parameter calculated from different schemes can yield some primary prediction of clustering formation, but its use must be accompanied with a lot of caution

- The minimum fluidization test was successfully conducted for FCC of average 80 μm size

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Thank You