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4	D4.4	Models for 1D Simulations of Packed beds	Authors: Arpit Singhal, Schalk Cloete, Stefan Radl	1.0	UCoimbra	Other	PU	30/06/2016	

Abstract

This work presents a modelling study of gas-particle heat transfer on two distinct scales. Firstly direct numerical simulations (DNS) are conducted in a geometry of spherical particles generated via the discrete element method (DEM). Simulations are completed on random particle arrays ranging from a void fraction of 0.9 to maximum packing over a range of Reynolds number. The geometry is meshed with a fine Cartesian cut-cell mesh both inside and outside the particles. These DNS results are then used to provide improved heat transfer closures to an unresolved Lagrangian modelling approach which can be used to simulate much larger particle beds. The unresolved Lagrangian approach also incorporates a 1D heat conduction model to directly simulate heat transfer inside the particles. This model is then verified against DNS data in geometries where wall effects and intra-particle heat transfer, both of which are directly accounted for by the Lagrangian approach, are important. These new heat transfer closures derived are applicable to infinitely large beds. The CFDEM simulations adjust these 1D closures for narrow geometries with a low D/d ratio. Minor differences in results are discussed and the achievable computational speedup by this approach is quantified.

Methodology

DEM (particle bed generation)

In this work ANSYS FLUENT and Design Modeler is used for DEM (Discrete Element Method) to generate the packed bed. The particles are injected in the reactor geometry without the gravity force and acting under the normal and tangential forces of collision due to overlap. After 20s of the translation and collision of the particles in the DEM simulation the resulting random packed bed of the particles is obtained.

Mesh

The packed bed reactor geometry is meshed with refined cutcell mesh using ANSYS Meshing both inside and outside the particles.

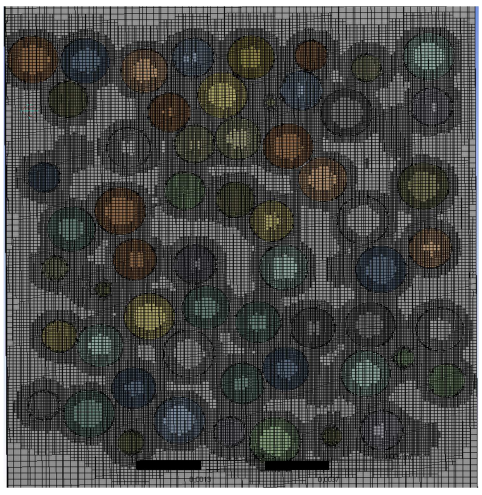


Figure 1: The section (y=0) of the reactor geometry with cutcell mesh

CFD (DNS)

ANSYS FLUENT is used to perform the DNS of the CFD part of the simulations.

Model equations

The conservation equations of continuity, momentum, and energy for the incompressible, steady state, Newtonian fluid solved for the DNS in this paper are given by

$$\nabla.\vec{u} = 0 \qquad (1)$$

$$\nabla.(\rho\vec{u}\vec{u}) = -\nabla p - \mu\nabla^2\vec{u} + \rho\vec{g} \qquad (2)$$

$$\rho C_p \nabla.(T\vec{u}) = K_f \nabla^2 T \qquad (3)$$

The particle equation of motion for the DEM simulations is given by:

$$m_P \frac{dv}{dt} = m_P g + \sum_{i=1}^{j}(F_{P,i,n} + F_{P,i,t}) \qquad (4)$$

Boundary conditions

The reactor is contained with a velocity inlet and pressure outlet. While the reactor walls are maintained at a condition of zero heat flux with no-slip condition. The particles contain a constant heat source of $1e^{07}$ W/m^3 integrated in the centre of all the cells inside the particles to obtain the correlation with heat source. In order to obtain the correlation with constant temperature particles are maintained at a fixed temperature of 573 K.

$$\varphi_{P\to f} = h \times (av.(T_P) - T_{bulk}) \qquad (5)$$

The heat transfer coefficient *(h)* is computed using the Eqn. (5), where (T_P) is the average for all the particle surface temperatures and (T_{bulk}) is the bulk fluid temperature.

Averaging procedure

Computation of the fluid temperature in the reactor is really important. The concept of the bulk fluid temperature (T_{bulk}) to obtain the heat transfer was used by Deen et al. suggesting that the fluid temperature should be computed on several planes in the direction perpendicular to the flow direction. While Sun et al. used the average fluid temperatures (T_{av}) to obtain the heat transfer predictions. Both these temperatures are used to formulate correlations and are verified against the unresolved model to obtain the correct averaging procedure.

The averaging procedures can be represented in form of the equations, with Eqn. (6) Eqn. (7) showing the bulk fluid temperature and average temperatures respectively; where T is the static fluid temperature:

$$T_{bulk} = \frac{\int (u.e_z) T \, dV}{\int (u.e_z) \, dV} \quad (6)$$

$$T_{av} = \frac{\int T \, dV}{\int dV} \quad (7)$$

Non-resolved Eulerian-Langrangian simulations

The non-resolved simulations involve the usage of the DEM open source package LIGGGHTS for generation of the packed bed, CFDEM-Coupling for the CFD simulations and PARSCALE for the intra particle temperature distributions. The CFD and DEM code generally perform their calculations separately in parallel and exchange data in accordance with the coupling intervals decided.

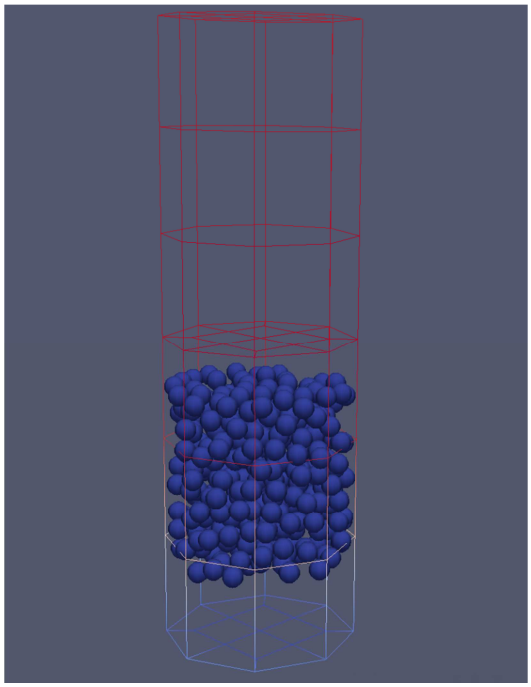


Figure 2: Non-resolved Euler-Langrangian grid setup

In non-resolved Euler-Langrangian simulations the particles are not resolved, which means that particle sizes are smaller than the computational grid (Figure 2), making the whole procedure of the simulation computationally cheaper than the resolved simulations.

The interaction of the particle phase with the fluid phase in terms of the momentum, energy and mass transfer is considered. This is facilitated by using the appropriate correlations to account for the transfer.

For example, to account for the external heat transfer, the correlations obtained in the following work are applied.

Results

Heat transfer in randomly arranged packed beds

The results for the heat transfer coefficient through spherical particles (with non-homogenous particle surface temperature) in the packed bed of different porosities simulated with different Reynolds numbers (Table 4) are benchmarked against the correlation results from Gunn et al., Deen et al. and Sun et al. Figure 3 shows the temperature variations with the change in Reynolds numbers and the porosity values. The temperature gradient inside the particle with different Reynolds number can be visualised.

The plots for the convective heat transfer inside the region of interest free from wall, inlet and outlet effects are shown in Figure 4, it is seen that the results agree significantly with the correlation values. The difference is due to the limitation in the existing correlations that they don't consider the gradient inside the particle. The heat transfer coefficients (h_{bulk} & h_{av}) are extracted using the bulk fluid temperature (T_{bulk}) and average fluid temperature (T_{av}) respectively.

Nusselt number correlation for the external heat transfer

The correlation for the external heat transfer from particle to fluid (Nusselt number) in the random packed bed with non-homogenous particle surface temperature and homogenous particle surface temperature are obtained, by fitting the data obtained over different porosities and Reynold numbers.

The effect of the change in Prandtl is not considered in this current correlation (*Pr = 1*). The correlation is valid over a porosity range ($0.4 < \varepsilon < 0.9$) and particle Reynolds number ($Re_p<100$).

The correlation is fitted in the structure of the Gunn correlation. Two different methods to compute the fluid temperature described previously are used to obtain different correlations according to the method of computing fluid temperature.

Correlations with non-homogenous particle surface temperature

The particles contain a constant heat source of $1e^{07}$ W/m^3 integrated in the centre of all the cells inside the particles.

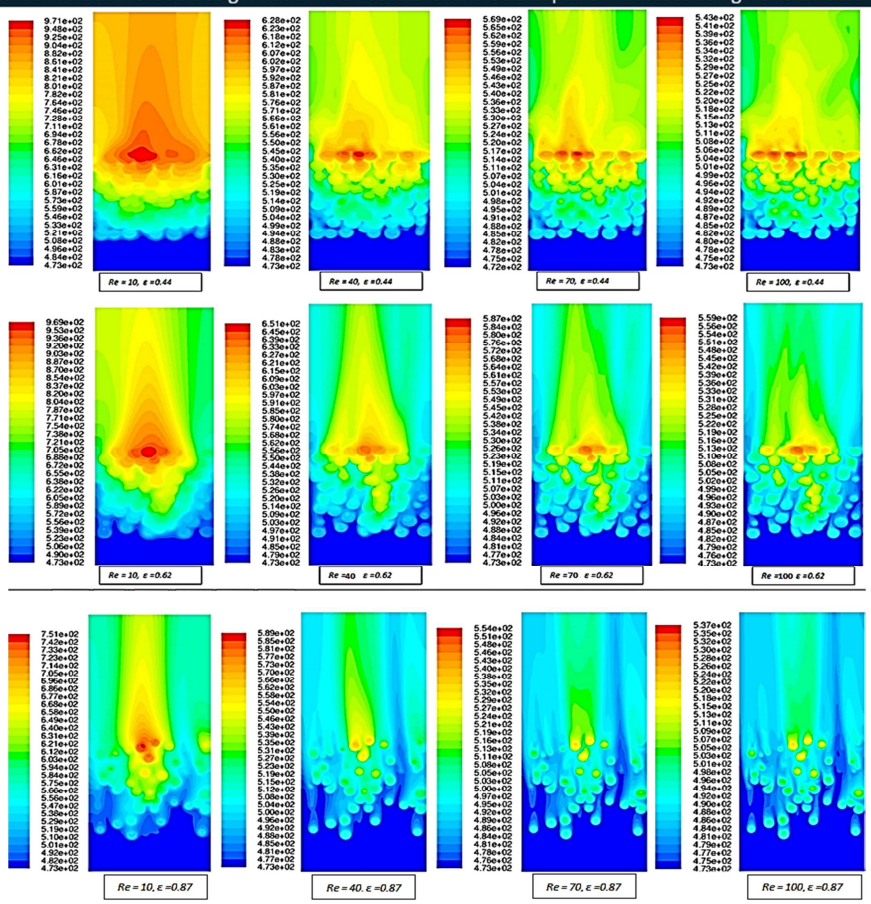


Figure 3: Temperature distribution profiles with temperature gradients inside the particles at plane y=0, through the reactor geometries with different Porosities and Reynolds numbers for the case with integrated heat source inside the particles

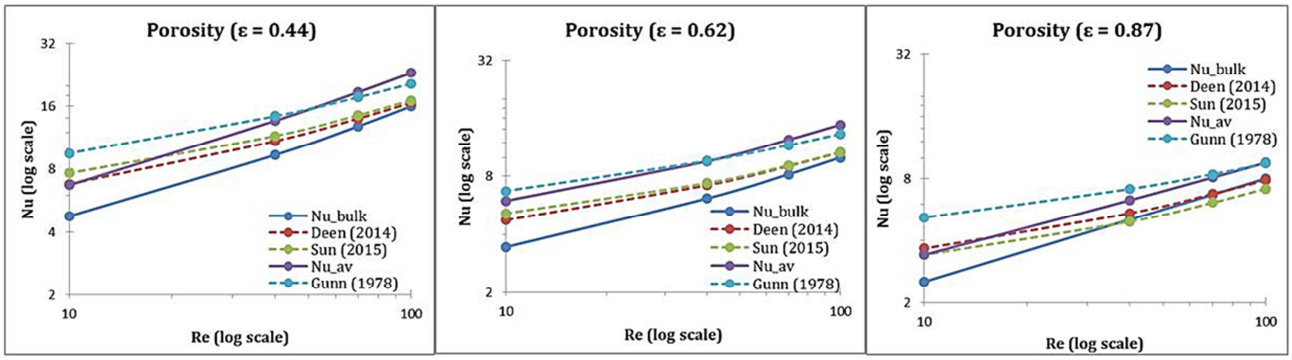


Figure 4: Comparison of the heat transfer coefficient in the region of interest *(no wall, inlet outlet effects)* over different porosity and Reynolds number values for the case with integrated heat source inside the particles

Using volume averaged and bulk fluid temperatures separately, the correlations obtained are

With volume averaged bulk fluid temperature

$$Nu = (0.455 + 5.09\varepsilon - 5.05\varepsilon^2)(0.67 + 0.35Re^{0.2}) + (1.73 - 3.38\varepsilon + 1.95\varepsilon^2)(Re^{0.7}) \quad (8)$$

With volume averaged fluid temperature

$$Nu = (-1.42 + 6.43\varepsilon - 5.12\varepsilon^2)(3.2 + 2.54Re^{0.2}) + (2.9 - 6.13\varepsilon + 3.59\varepsilon^2)(Re^{0.7}) \quad (9)$$

Correlations with homogenous particle surface temperature

The particles are fixed at a constant temperature 573K. The correlations for this case setup are obtained with both averaged and bulk fluid temperature.

With volume averaged bulk fluid temperature

$$Nu = (2.844 - 3.49\varepsilon + 2.36\varepsilon^2)(-0.71 + 1.17Re^{0.2}) + (1.4 - 2.35\varepsilon + 1.12\varepsilon^2)(Re^{0.7}) \quad (10)$$

With volume averaged fluid temperature

$$Nu = (-0.3 + 6.87\varepsilon - 6.31\varepsilon^2)(-1.08 + 2.60Re^{0.2}) + (2.28 - 4.58\varepsilon + 2.51\varepsilon^2)(Re^{0.7}) \quad (11)$$

The validity of these correlations is determined with the help of unresolved Euler-Langrangian model. The results are used to determine the best method to determine the fluid temperature.

Comparison of the correlations with non-homogenous vs homogenous particle temperature

As described in previously, correlations are obtained with both non-homogenous and homogenous particle surface temperatures. The comparison for the prediction of heat transfer with both the correlations is thus studied with different Reynolds numbers and porosities. Figure 5 shows the significant change in prediction of heat transfer is observed for higher porosities. Which is because at higher porosities the boundary layer formed around the particles is thicker and thus the heat transfer gets affected significantly by the particle surface temperature (whether it is homogenous or non-homogenous).

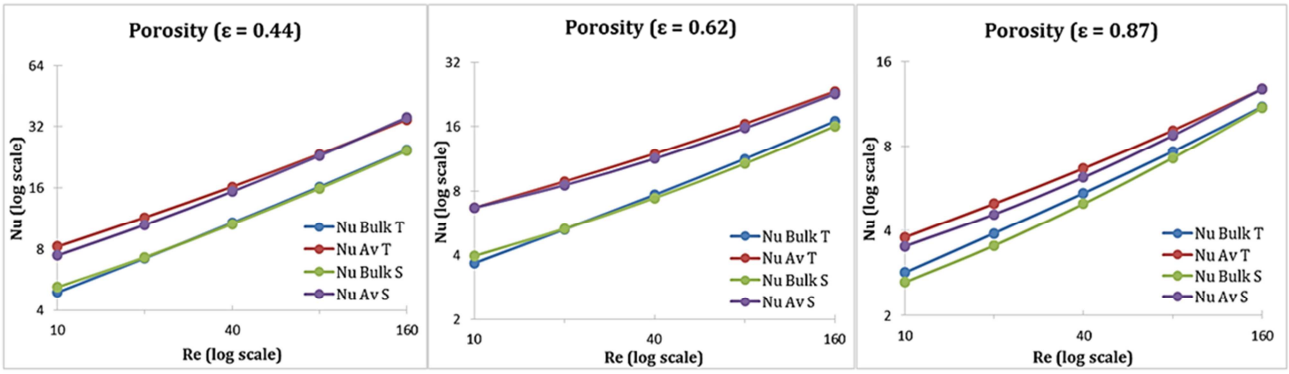
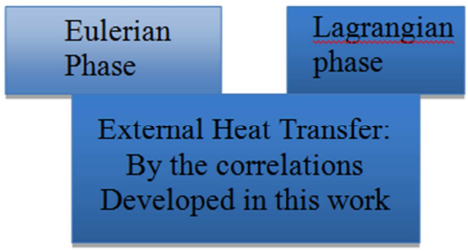


Figure 5: Comparison of the prediction of heat transfer from the correlations obtained in this work. (*Where, T = constant temperature (homogenous particle surface temperature); and S = integrated heat source (non-homogenous particle surface temperature*)

Comparison between the resolved and unresolved model

The correlation obtained with homogenous particle surface temperature is used to account for the external heat transfer in the non-resolved Euler-Langrangian simulations. The particle bed with a porosity of 0.62 is replicated in LIGGGHTS® + CFDEM® + PARSCALE® simulation, with identical flow properties as in the PR-DNS using FLUENT.



i) Mean particle surface temperature

This is the comparison of mean particle surface temperatures over different Reynolds number (Figure 6). The approximation is quite reasonable. Only at low Reynolds number the difference can be observed which we can be speculated looking into the later results.

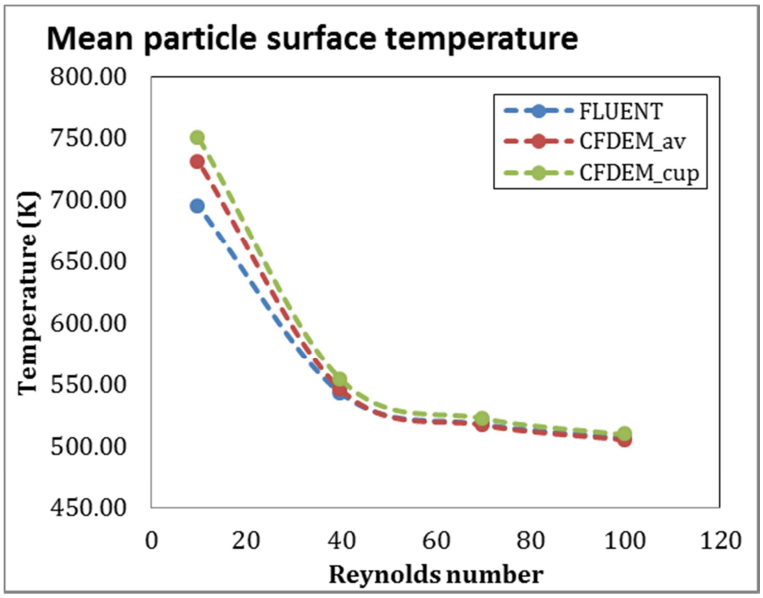


Figure 6: Comparison of the prediction of mean particles surface temperature from PR-DNS and non-resolved simulations. (*Where, FLUENT= Prediction from PR-DNS; and CFDEM_av and CFDEM_cup are predictions from non-resolved simulations with averaged fluid temperature and bulk fluid temperature respectively)*

ii) Fluid Temperature profiles

This is the comparison of the fluid temperature profiles obtained from CFDEM and FLUENT, the temperature profile match quite well and the CFDEM approach is able to predict fluid temperature reasonable well when compared with PR-DNS results from FLUENT. The grid for the unresolved setup was refined to the point to obtain a grid independent result and to be able to capture the effects to the level of particle scale.

The results show the overall temperature for Re10 is higher and the prediction is not in agreement with FLUENT result, which is seen in the mean particle surface temperature predictions as well.

iii) Intra-particle temperature distributions

With the presence of PARSCALE coupled to our unresolved simulation we can obtain the 1D profile for the variation of temperature inside the particle (radial). In here we compare the distribution inside the particle given by 1D code PARSCALE® (symmetric profile) and FLUENT (asymmetric profiles).

For the comparison the particles chosen for the study are seen in the Figure 8. One particle is chosen from the top of the bed, while one from the bottom of the bed. Three different particles are considered in the middle of the bed, each representing different temperature zones.

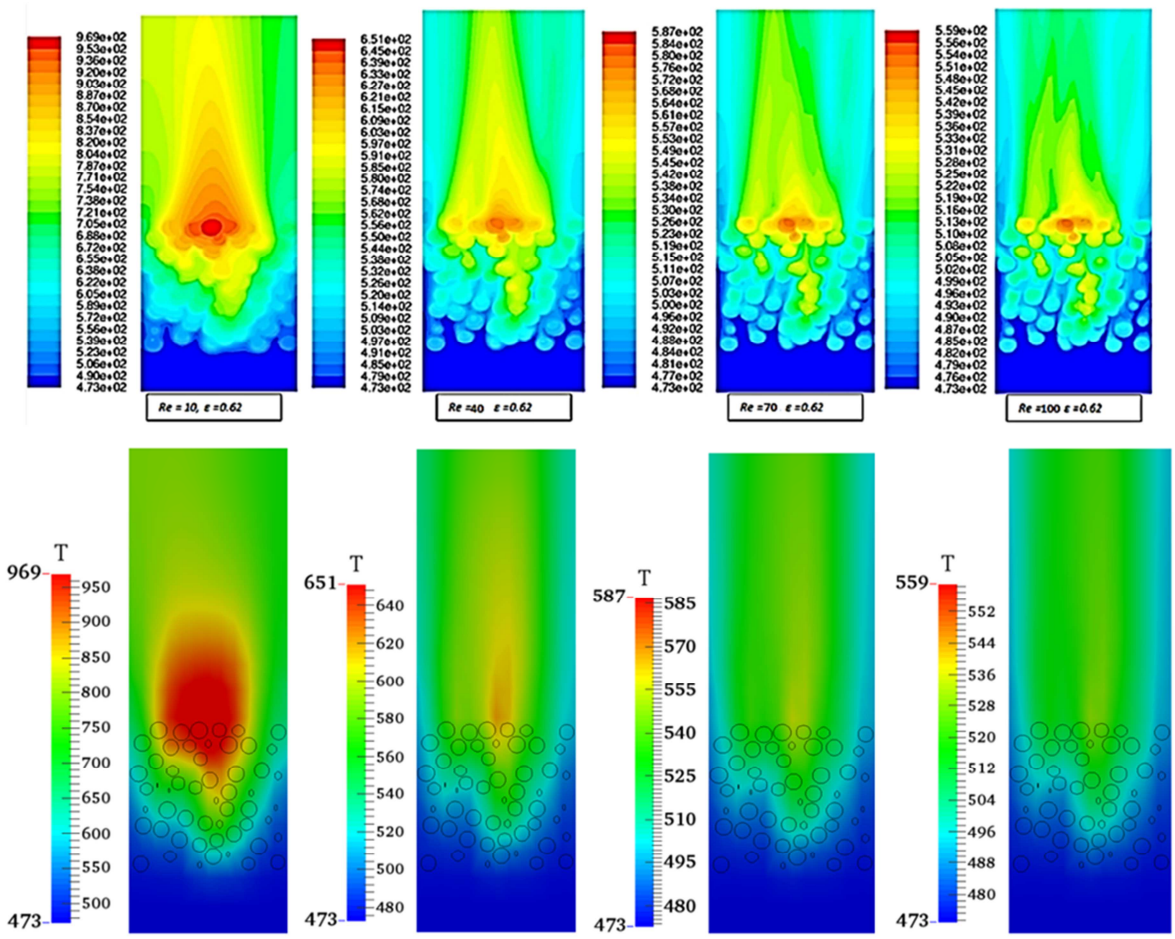


Figure 7: *Temperature distribution profiles at plane y=0, through the reactor geometries with different and Reynolds numbers for the case with a fixed volumetric heat source inside the particles. FLUENT (above) and CFDEM (below)*

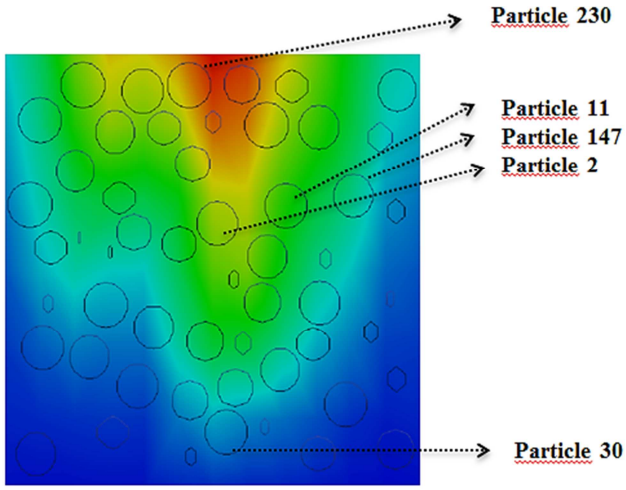
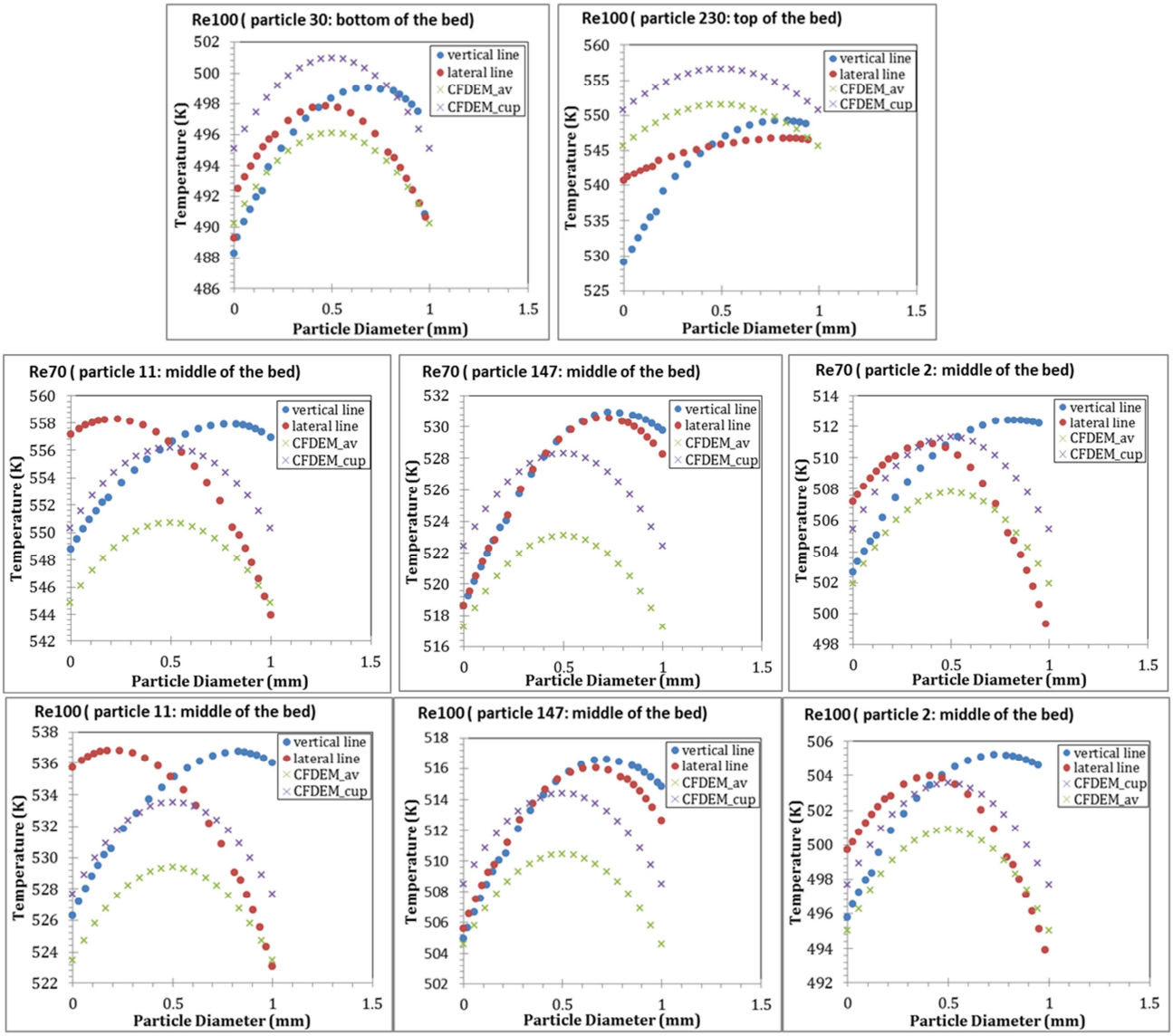


Figure 8: *Approx. location of the particles studied for the intra particle temperature distribution comparison*

In the plots shown in Figure 9, the intra particle temperature distributions obtained for particles represented in Figure 8 can be seen for Re100. The predictions at Re100, suggests really good match with the results from PARSCALE®, considering the fact that the results obtained with FLUENT are asymmetric in nature.

Similar predictions are observed for Re70 and 40 shown in Figure 9. The variation in prediction of intra particle temperature is similar to PR-DNS results from FLUENT. The predictions with average and bulk fluid temperatures don't show a huge difference. Both the correlations predict the temperatures equally well.



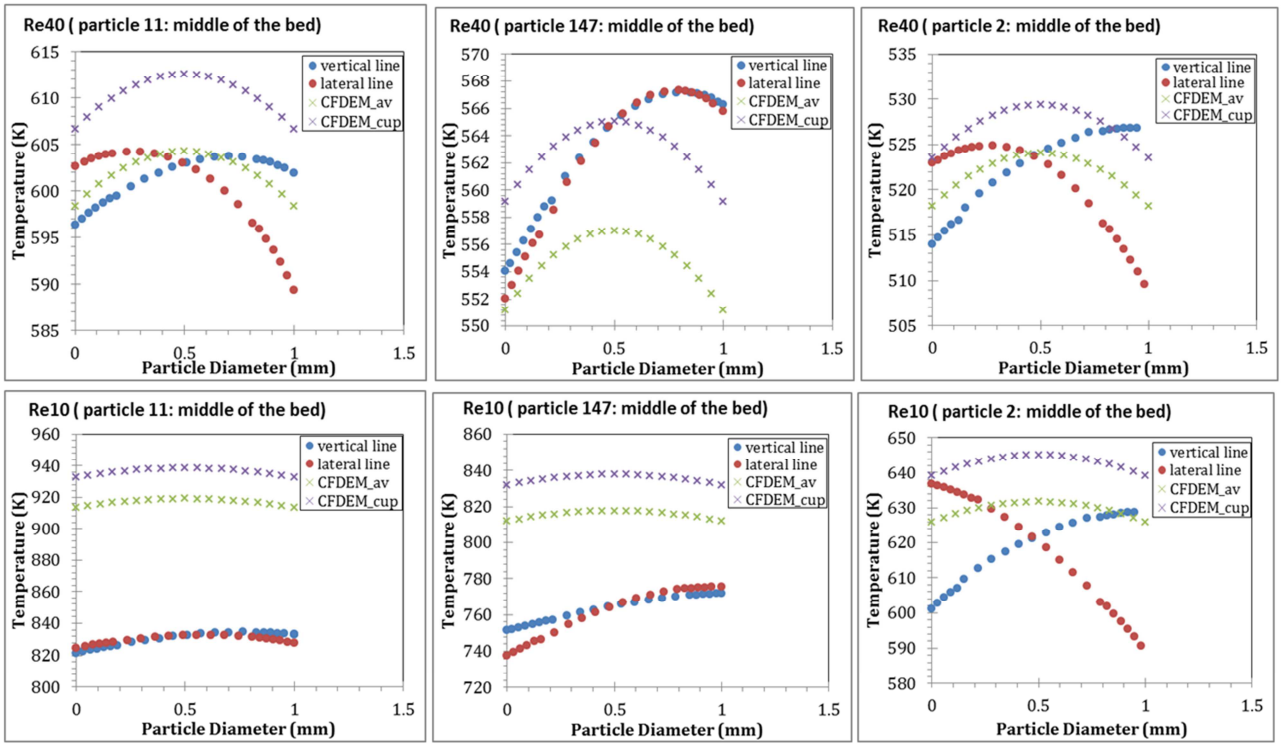


Figure 9: *Intra particle Temperature distribution profiles at Re100, Re70, Re40 and Re10 obtained from FLUENT (asymmetric) and PARSCALE (symmetric). [Vertical line = prediction in the direction of flow (FLUENT), Lateral line= prediction perpendicular to the flow (FLUENT); CFDEM_av and CFDEM_cup = PARSCALE predictions in a non-resolved coupled simulation using different fluid averaged temperatures (average and bulk fluid respectively)].*

At Re10, the heat transfer will be very fast therefore there will not be a gradient between the surface temperature and the center temperature of the particle. The deviation is observed at Re10, which was seen in Figure 6, Figure 7 and also in Figure 9. But at low-Reynolds number the mean particle temperature will be generally higher. Moreover models at low-Reynolds number and Pr ~ 1 are difficult to determine, because the heat transfer is very fast. It is clear that any model for this regime has more inaccuracies than models for larger Re. Therefore having a heat transfer model for such low Re might not be necessary and industrial scale packed bed reactors doesn't operate at such low Reynolds number.

iv) Nusselt Number with wall distance

To obtain a clear picture of the presence of wall effects, a Nusselt number with wall distance variation plot is obtained as shown in Figure 10 at Reynolds number (Re100) with the unresolved approach mentioned above. The cluster plot shows the presence of high Nusselt number near the wall of the reactor and then becomes quite stabilized within $d_p/2$ distance. For now we can only report from the unresolved approach (COSI platform) because FLUENT imposes the current limitation in extracting the per particle Nusselt number.

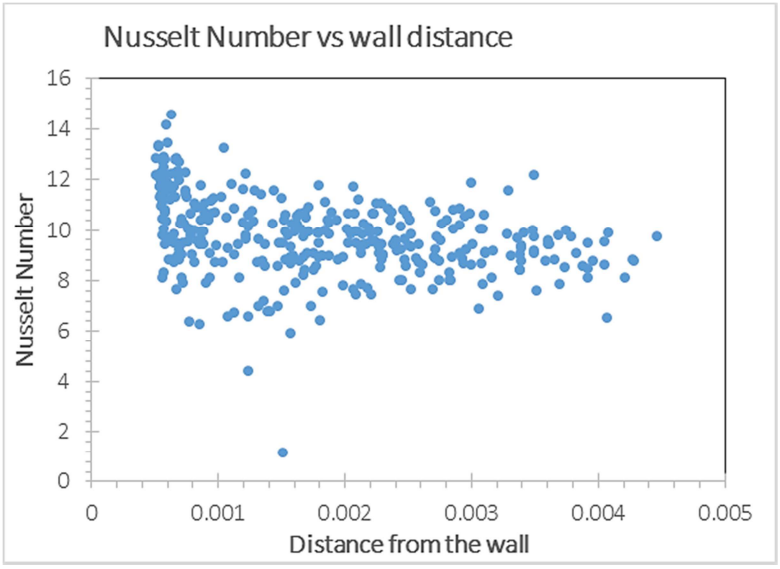


Figure 10: *Nusselt number variation with the wall distance for Re100 obtained from the unresolved simulation approach*