Development of Continuous Random Walk model based on normalized Langevin equation in OpenFOAM for turbulent dispersion and validation against DNS statistics

M. Kampili[1], S. Kelm[1], A. Dehbi[2], H.-J. Allelein[1]

[1]Institute for Energy and Climate Research IEK-6, Forschungszentrum Jülich GmbH, Wilhelm-Johnen-Straße, 52428, Jülich, Germany, +49 2461 61 4075
[2]Laboratory for Scientific Computing and Modeling, Paul Scherrer Institute, Forschungsstraße 111, 5232, Villigen, Switzerland
m.kampili@fz-juelich.de

Introduction:

Aerosol transport plays a significant role in many industrial, medical and environmental flows. For example, a few major applications are pollutants transport, drug delivery in respiratory system and fouling of turbine blades. Often, modeling of turbulent dispersion of particles plays considerable role in predicting particle motion and deposition due to the wall shear turbulence in industrial flows.

In the recent years, OpenFOAM had become a powerful toolkit for CFD simulations because of the large number of numerical methods available, flexibility and the transparency of the open-source code. The Lagrangian Particle Tracking has considerable applications in automobile, chemical and process industries. For instance, particularly using OpenFOAM, particle/droplet transport in IC engines [1], cyclone separators [2] are simulated. The in-built model available for modeling turbulent dispersion is based on Discrete Random Walk (DRW) approach from Gosman and Iodinnes [3]. This model predicts the particle dispersion with reasonably good accuracy in case of homogeneous and isotropic turbulence.

In most of the industrial applications, flow turbulence is non-homogenous and anisotropic close to the walls. Because of the isotropic turbulence assumption in DRW model, this model over-predicts deposition of particles even in simple flows such as turbulent pipe flow [4, 5]. The over deposition of particles is due to the high wall normal turbulent dispersion velocity predicted in the model. Improved DRW models are proposed by Matida [6], Dehbi [4] by using a correction for wall normal dispersion velocity and using DNS correlations for RMS velocities in the boundary layer. There were efforts to implement the model of Matida in OpenFOAM [7]. The implementation of DRW and improved DRW models in OpenFOAM is documented in detail by Jundi [7].

In spite of considering anisotropy in the boundary layer, DRW model fails to predict the particle dispersion when there is strong inhomogeneity of turbulence in the flow. The best results for particle dispersion in turbulent pipe flows are obtained by Parker et al. using RSM models for turbulence modeling [5] which account for anisotropy of turbulence in boundary layer. In spite of all these improvements, DRW models pose sudden change in particle velocities leading to infinite acceleration due to inherent modeling deficiency and fails in case of nonhomogeneous turbulence field.

In the side line, the models for Brownian diffusion are developed based on Langevin equation. A similar approach based on Langevin equation has been followed to develop models for turbulent dispersion. These models are often called Continuous Random Walk (CRW) models in literature. First implementation of basic CRW model in OpenFOAM and the evaluation of the turbulence dispersion and particle transport in cyclone separator have been performed by Jang et al [2].

There was a significant improvement in the CRW modeling by normalizing the Langevin equation with rms of velocities and hence better results for predicting turbulent dispersion by Thompson et al (1984) [8]. Bocksell and Loth developed further to make it suitable for inertial particles by adding a correction to drift correction term [9]. Dehbi extended this model to arbitrary geometries by including local and global coordinate system transformations [10]. Fortunately, this model predicts the turbulent dispersion accurately even in the case of inhomogeneous turbulence due to the presence of drift correction terms in governing equations.

In the present paper, the focus is on implementing CRW model based on normalized Langevin equation applicable for arbitrary geometries in OpenFOAM-6 and validating in a detailed manner using DNS velocity statistics available for the particle transport in turbulent channel flow by Marchioli et al [11]. In the DNS simulations considered for reference, a fully developed channel flow with periodic boundary conditions is simulated. However in the present simulations, a long 2D channel flow has been considered with inlet and outlet, and the fully developed region is used for particle tracking. The results from OpenFOAM-6 are compared with existing literature [12], which provides a code to code verification with Ansys Fluent particle tracking and the UDF implementation of CRW model. This model implementation is developed under the frame work of our in-house tailored CFD solver “containmentFoam” for nuclear containment flow applications [13].

CFD Model:

Channel flow:

Fully developed turbulent channel flow (Re_τ = 150) is simulated using RANS equations closed by k-ω SST model. Channel width is 300 non-dimensional wall units (y+), and the length of 5 m is considered so that all the particles reside in domain throughout the simulation time. For further details, please refer to the article on DNS simulations of particle transport in fully developed channel flow by Marchioli et al [11].

Lagrangian Particle Tracking:

It is assumed that dispersed particle phase is dilute enough that one way coupling is sufficient. Particle size ranges from 7.68 microns to 192 microns, which leads to particle relaxation time ranging from 0.2 to 125. Statistically sufficient number of particles (10000 in this case) are injected uniformly in the cross section at the start of fully developed region. Particles are tracked in a fixed fully developed turbulent flow field. Particles are assumed to rebound perfectly elastic at the walls. The fully developed region is entirely comprised of boundary layer and hence turbulence is inhomogeneous in the wall normal direction.

Governing equations for particle motion:

Particle motion is tracked by using the time integration of Newton's second law. In the present simulations, drag force acting on the particles is considered, while all other forces are neglected. Lift force is negligible because of very high density ratio between particle and fluid. Brownian motion is not considered as the minimum particle size is above 1 micron. Gravitational force is found to have no effect on the velocity statistics [11] and it is not considered in present simulations.. Virtual mass and Pressure gradient forces are of second order in the present simulations. All these assumptions reduces the particle equation of motion to

$$m_p \frac{du_p}{dt} = F_D$$

Where m_p is particle mass, *up* is particle velocity, *t* is time and F_D is drag force acting on the particle. Drag force in OpenFOAM is modelled according to Schiller and Neumann (1933) as following.

$$F_D = C_D \frac{\pi D_p^2}{8} \rho_f (u_f - u_p) \left| u_f - u_p \right|$$

C_D is drag coefficient, D_p is particle diameter, ρ_f is fluid density and u_f is fluid velocity. Drag coefficient is defined as a function of particle Reynolds number.

$$C_D = \begin{cases} \frac{24}{Re_p}\left(1 + 0.15 Re_p^{0.687}\right) & if\ Re_p \leq 1000 \\ 0.44 & if\ Re_p > 1000 \end{cases}$$

Even though this formulation is different from commercial code Fluent, Griefzu et al confirmed that they result in same predictions for particle tracking [14]. The turbulent dispersion is modelled by modifying the fluid velocity u_f in equation 1 as u_f (mean) + *UTurb*. u_f mean is interpolated at the particle positon from mean velocity field, and the *UTurb* is predicted from CRW model as *(u_1, u_2, u_3)* described in next section.

CRW Model for turbulent dispersion:

In this section governing equations for predicting fluctuating velocity field along a particle track are presented briefly. Following Dehbi [10], normalized Langevin equations in boundary layer can be written as following:

$$\mathrm{d}\left(\frac{u_1}{\sigma_1}\right) = -\left(\frac{u_1}{\sigma_1}\right)\cdot\frac{\mathrm{d}t}{\tau_1} + \sqrt{\frac{2}{\tau_1}}\cdot\mathrm{d}\xi_1 + \frac{\partial\left(\frac{\overline{u_1 u_2}}{\sigma_1}\right)}{\partial x_2}\cdot\frac{\mathrm{d}t}{1+Stk}$$

$$\mathrm{d}\left(\frac{u_2}{\sigma_2}\right) = -\left(\frac{u_2}{\sigma_2}\right)\cdot\frac{\mathrm{d}t}{\tau_2} + \sqrt{\frac{2}{\tau_2}}\cdot\mathrm{d}\xi_2 + \frac{\partial\sigma_2}{\partial x_2}\cdot\frac{\mathrm{d}t}{1+Stk}$$

$$\mathrm{d}\left(\frac{u_3}{\sigma_3}\right) = -\left(\frac{u_3}{\sigma_3}\right)\cdot\frac{\mathrm{d}t}{\tau_3} + \sqrt{\frac{2}{\tau_3}}\cdot\mathrm{d}\xi_3$$

In the above governing equations, u_1, u_2, u_3 are velocity fluctuations in stream wise, wall normal and span wise directions, while σ_1, σ_2, σ_3 are rms of velocity (in respective directions) curve fitted from DNS data as shown in figure 1. The $d\xi$ represents random number from Gaussian distribution with zero mean and dt variance. The drift correction terms (third term in stream wise direction and wall normal direction) is obtained by curve fitting the DNS data obtained as in Dehbi 2010 [12].

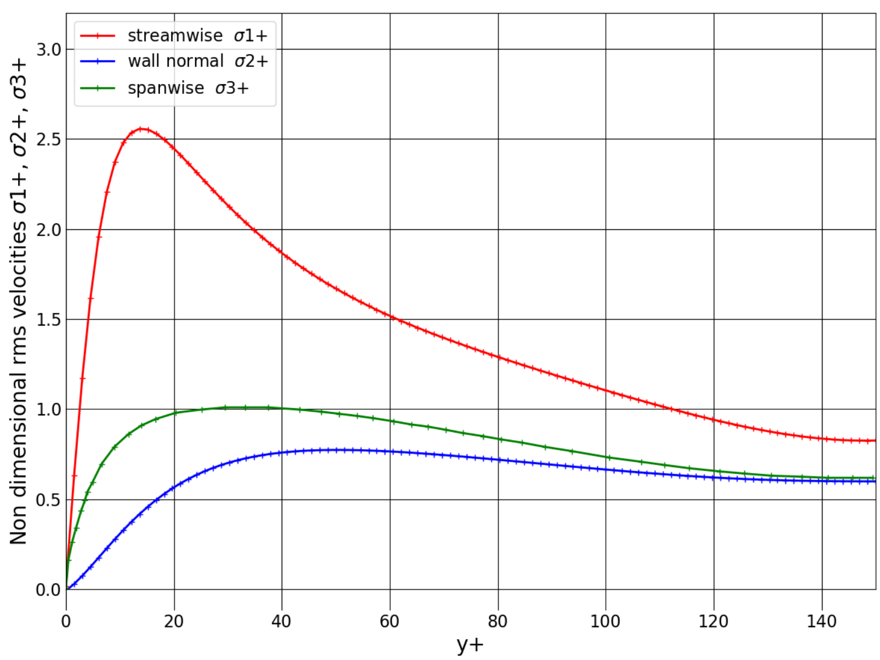

Figure 1: The rms of velocities in streamwise (1), wall normal (2) and spanwise (3) directions

Time scales in the flow in different directions are represented with τ_1, τ_2, τ_3 and they are assumed to equal. Time scales are computed using correlations from Kallio and Reeks [15] as following:

$$\tau_i = 10\frac{\nu}{u_\tau^2} \qquad\qquad y^+ \le 5$$

$$\tau_i = (7.122 + 0.5731\, y^+ - 0.00129\, {y^+}^2\,)\ \frac{\nu}{u_\tau^2} \qquad\qquad 5\ \le y^+ \le 200$$

Where v is kinematic viscosity of fluid and u_τ is friction velocity of turbulent channel flow. The *Stk* (stokes number) is defined as the ratio between particle relaxation time and flow time scale.

$$Stk = \frac{\tau_p}{\tau_i}$$

$$\tau_p = \frac{\rho_p d_p^2}{18\,\mu} \qquad when\ Re_p \le 1$$

$$\tau_p = \frac{4\,\rho_p d_p}{3\rho_f C_D\,\left|u_f - u_p\right|} \qquad when\ Re_p > 1$$

Implementation in OpenFOAM:

In OpenFOAM, a Face to Face algorithm is used to move the particles from initial position to final position in a Lagrangian time step. This poses fewer constraints on Lagrangian time step of particle motion, and hence no handle is provided to specify Lagrangian time step in OpenFOAM-6 [1]. Since the CRW model is dependent on the Lagrangian time step, another limit on time step is included as a function of particle relaxation time.

Additionally, `random` class in OpenFOAM-6 is used to calculate the random numbers needed in this model. First order Euler implicit numerical integration methods available in OpenFOAM-6 is utilized for all the governing equations of CRW model. Coordinate transformation from global to local [10] is implemented to make the code suitable for arbitrary complex geometries.

Results:

According to Dehbi 2010, this model not only predicts the particle deposition correctly but also provided deep insight into particle motion statistically. The particle velocity statistics are pretty close to the DNS data, though the flow field is predicted using RANS equations. In the present paper, code-to-code verification is performed by comparing the results of OpenFOAM-6 and Fluent. For the specification of particle inertia relative to fluid flow, non-dimensional relaxation time τ+ is defined as following:

$$\tau^+ = \frac{\tau_p u_\tau^2}{\nu}$$

The tracking time is also non-dimensionalized in similar manner as

$$t^+ = \frac{t\, u_\tau^2}{\nu}$$

To cover the particles in different regimes, non-dimensional relaxation times of 0.2, 5, 25 and 125 are considered for simulation. In figure 2, velocity statistics for τ+ 0.2 and 25 are presented in comparison with Dehbi 2010 [12]. From this comparison, it can be concluded that OpenFOAM-6 results are in good agreement with Fluent - UDF results.

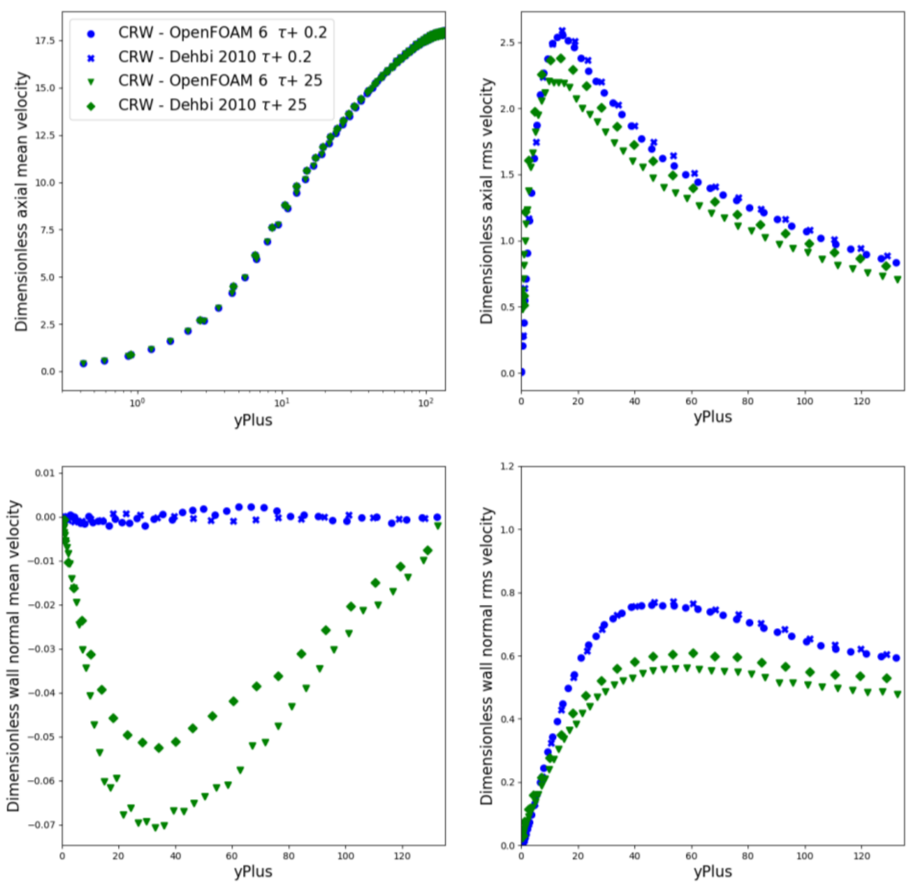

Figure 2: Velocity statistics comparison for τ+ 0.2 and τ+ 25 particles

The results are slightly different due to minor differences between OpenFOAM-6 and Fluent, such as not considering the particle radius when it is rebounding from wall. Another fundamental reason could be algorithms difference in Particle Tracking such as “Face to Face” and “Lose and Find”. These minor deviations are acceptable considering the accuracy of model predictions.

In the figure 3, particles distribution for τ+ 0.2 (very low inertia) in the channel width is computed and compared against the DNS data at different times. The channel is divided into 51 bins parallel to length following the bin width specification from Marchioli et al [11]. From the plots, it is concluded that the current model implementation is able to predict low inertial particles which are well mixed in the starting remain well mixed in spite of turbulent dispersion in turbulent flows.

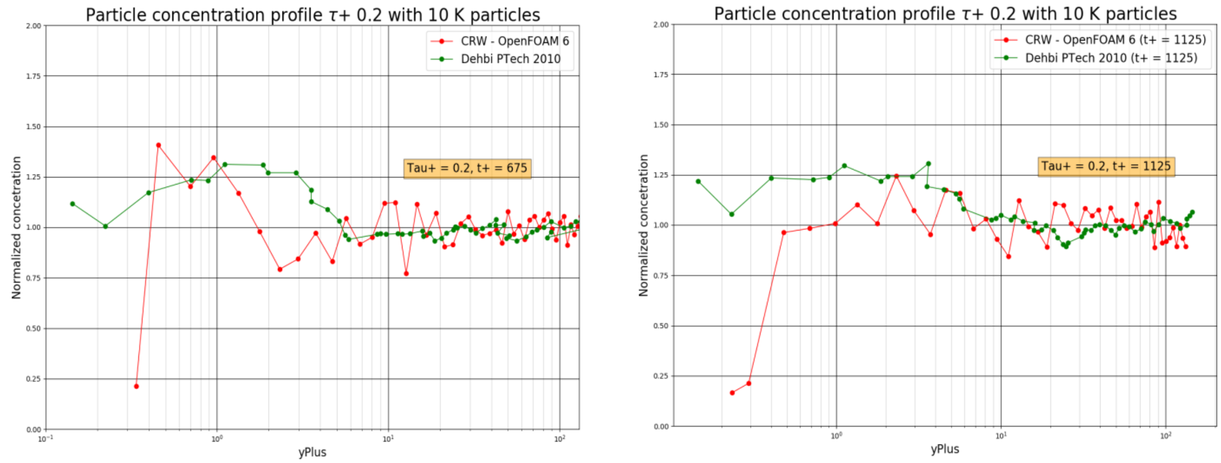

Figure 3: Particles (τ+ 0.2 at t+ 675, t+ 1125) distribution in the bins

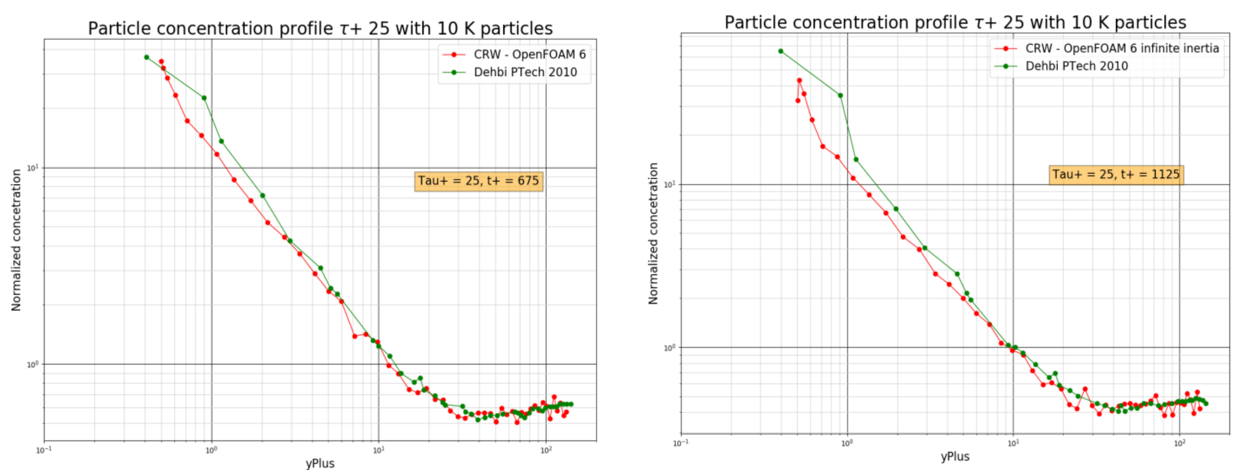

Figure 4: Particles (τ+ 25 at t+ 675, t+ 1125) distribution in the bins

In the literature, it is reported that when the particle inertia is high, particles tend to aggregate close to the walls. From figure 4, this expectation from the model implementation is verified for particles of τ+ 25 at two different times (t+ 675 and t+ 1125).

The deviation in figure 3 and figure 4 in the first bin of the channel width is due to the rebound boundary condition in OpenFOAM-6. In OpenFOAM-6, particles are rebounded when the particle center hits the wall, but physically particle center can't reach wall due to particle radius. Due to this minor deficiency in the boundary condition, there are ~5% of particles are trapped additionally in the first few bins. In Fluent, the particle gets rebounded when the particle surface hits the wall. This is a fundamental difference in boundary condition between OpenFOAM-6 and Fluent.

Improvements over DRW results:

Velocity statistics for τ+ 0.2 with Discrete Random Walk (DRW) model are compared with Continuous Random Walk (CRW) model results in Figure 5. It clearly shows the improvement for both particle velocity mean values and rms values, as CRW model predictions are matching with predictions of Dehbi 2010 [12] and Marchioli DNS data [11]. The most important one is the prediction of wall normal mean velocity for engineering applications, because it directly affects the particle deposition as well as the particle concentration distribution. RMS of particle fluctuation velocities are significantly under predicted with default DRW model in OpenFOAM-6.

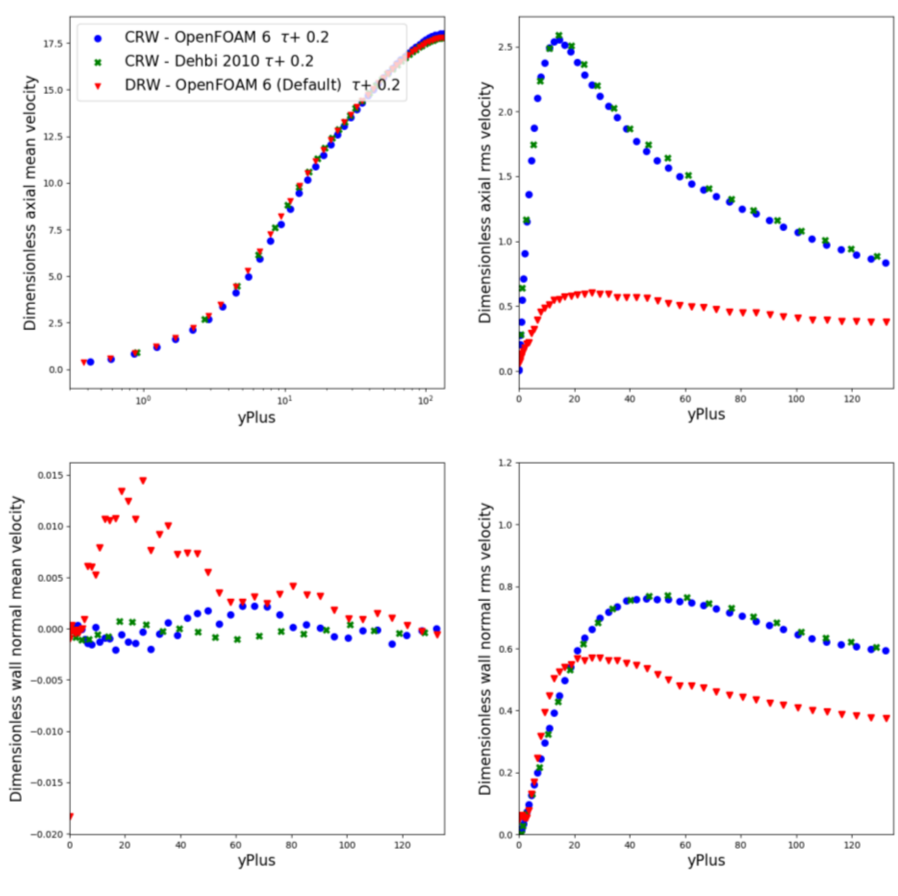

Figure 5: Comparison of velocity statistics for τ+ 0.2 with CRW and DRW

Summary and future work:

In the present paper, default Discrete Random Walk model in OpenFOAM is discussed along with efforts in OpenFOAM community to implement improved DRW model by Matida et al. Recently there was attempt made by Jang et al (2018) to implement and validate the CRW model based on Langevin equation in OpenFOAM. In the current work, the need to implement CRW model based on normalized Langevin equation is emphasized due to significant improvements in the modeling approach by Thompson, Bocksell and Loth, and Dehbi. To verify the model implementation, a standard channel flow problem is chosen for which detailed DNS statistics and also Fluent – UDF results are available [Dehbi]. The model intricacies and its implementation in OpenFOAM are discussed to identify the fundamental differences between OpenFOAM and Fluent Lagrangian Particle Tracking algorithms such as handle on the Lagrangian integration time step. Code to code verification is performed by comparing the results presented for selected particle sizes with $\tau+$ 0.2 and $\tau+$ 25. Velocity statistics of the particles as well as the distribution of particles across the channel width are compared with existing literature data from Dehbi 2010 [12]. The reason for deviation of the particle concentration in the first bin is identified as the `rebound` boundary condition for particles. The results predicted with our implementation of CRW in OpenFOAM-6 are in good agreement with Dehbi 2010 [12] and Marchioli et al [11]. Well mixed criteria for low inertial particles ($\tau+$ 0.2) and particle aggregation in the boundary layer for high inertia particles ($\tau+$ 25) are predicted with reasonable accuracy. Finally, the improvement in the results due to modeling choice (DRW or CRW) is clearly shown, by direct comparison of velocity statistics for $\tau+$ 0.2 with DRW and CRW.

For the final presentation in conference, it is possible to include the results of particle deposition simulations at Reynolds numbers 10000 and 50000 in 3D geometries. A detailed validation against experimental data will be presented for the same, along with the results from default turbulent dispersion model in OpenFOAM-6. Due to the availability of number of `postProcessing` function objects and continuous development of OpenFOAM from ESI group, there is also an ongoing work to develop these models in OpenFOAM-v1812. The plan for transferring code to higher versions of OepnFOAM, advantages and difficulties, as well as the results from OpenFOAM –v1812 could be expected in the final presentation.

Future recommendations for OpenFOAM development: Rebound with radius BC, re-injection of particles, Handle on Lagrangian time step in dictionary.

References:

1. Niklas Nordin. P. A, “Complex chemistry modeling of diesel spray combustion”, *PhD Thesis at Chalmers University* (2001).

2. Jang. K et al, “Evaluation of the turbulence models for gas flow and particle transport in URANS and LES of a cyclone separator”, *Computers and Fluids*, 172, 274-283 (2018).

3. Gosman. A. D et al, “Aspects of computer simulation of liquid fueled combustors”, *Journal of Energy*, 7, 482 – 490 (1983).

4. Dehbi. A, “A CFD model for particle dispersion in turbulent boundary layer flows”, *Nuclear Engineering and Design*, 238, 707-715 (2008).

5. Parker. S et al, “Towards quantitative prediction of aerosol deposition from turbulent flows”, *Journal of Aerosol science*, 39(2), 99-112 (2007).

6. Matida. E. A et al, “Improved numerical simulation of aerosol deposition in an idealized mouth–throat”, *Journal of Aerosol Science*, 35, 1-19 (2004).

7. Jundi. X, “Modification of Stochastic Model in Lagrangian Tracking Method”, *In Proceedings of CFD with OpenSource Software*, Edited by Nilsson .H, (2016).

8. Thompson. D. J, “Random walk modeling of dispersion in inhomogeneous turbulence”, *Quarterly Journal of the Royal Meteorological Society*, 110(466), 1107 – 1120 (1984).

9. Bocksell. T. L et al, “Stochastic modeling of particle diffusion in a turbulent boundary layer”, *International Journal of Multiphase Flow*, 32, 1234 – 1253 (2006).

10. Dehbi. A, “Turbulent particle dispersion in arbitrary wall-bounded geometries: A coupled CFD-Langevin-equation based approach”, *International Journal of Multiphase Flow*, 24, 819-828 (2008).

11. Marchioli. C et al, “Influence of gravity and lift on particle velocity statistics and transfer rates in turbulent vertical channel flow”, *International Journal of Multiphase Flow*, 33, 227-251 (2007).

12. Dehbi. A, “Validation against DNS statistics of the normalized Langevin model for particle transport in turbulent channel flows”, *Powder Technology*, 200, 60-68 (2010).

13. Kelm. S et al, “Development and First Validation of the Tailored CFD Solver ‘containmentFoam’ for Analysis of Containment Atmosphere Mixing”, *International Topical Meeting on Nuclear Reactor Thermal Hydraulics (NURETH-18)* in Portland, Oregon, USA (2019).

14. Greifzu. F et al, “Assessment of particle-tracking models for dispersed particle-laden flows implemented in OpenFOAM and ANSYS FLUENT”, *Engineering Applications of Computational Fluid Mechanics*, 10(1), 30-43 (2016).

15. Kallio. G. A et al, “A numerical simulation of particle deposition in turbulent boundary layers”, *International Journal of Multiphase Flow*, 3, 433 – 446 (1989).