Mesh parameters:

Fr	: Boundary layer first row size (mm)
R	: Boundary layer growth factor
Nr	: Boundary layer number of rows
Nn	: Circular resolution
Nns	: Core radial resolution in front of the sphere
GF	: Core radial growth factor in front of the sphere
Ndc	: Core axial resolution in front of the sphere
GD	: Core axial growth factor in front of the sphere
Nps	: Axial resolution above the sphere
Ndp	: Tube radial resolution
Fl	: Tube radial inner first row size (mm)
Fn	: Tube radial outer first row size (mm)
Npi	: Inlet axial resolution
Ll	: Inlet axial last row size in mm

Introduction

Developed by a team led by South Africa, a new concept of nuclear reactor named Pebble Bed Modular Reactor should be able to offer high efficiency production of electricity and better safety performances than the actual fusion reactors. As part of this project, the department of Nuclear Energy and Safety (NES) of the Paul Sherrer Institut contributes to the development of computational methods to predict the progression of severe accidents and the release of radioactive materials into the atmosphere.

The Pebble Bed Modular Reactor (PBMR) is an advanced high-temperature gas-cooled, and graphite moderated reactor. The fuel elements are spherical graphite “pebbles” about 6 cm in diameter. These spheres contain microsphere of uranium dioxide. Helium gas flows over and through the gaps between the pebbles and act as a coolant. The graphite fuel has high thermal conductivity and high heat capacity. Because of that, the plan can withstand a broad spectrum without the need for operation of active safety systems and with very limited release of radionuclides to the environment. Nevertheless, in the PBMR design, the graphite pebbles are continually rubbing against each other. Because of that a very large quantity of graphite dust is released in the reactor coolant system. Then dust particles are transported and deposed on surfaces by aerosol processes. Thus, in the event of a pipe leak, rapid depressurization of the system may cause the release of radioactive material airborne into the surrounding atmosphere. That’s why it is very important to develop computational models witch quantify accurately the potential threat of these radioactive aerosols, and the Laboratory of Thermal-Hydraulic (LTH) of the NES contributes to such project. A part of the development of such models consists on modeling the aerosol deposition rate on pebble bed during normal and critical operating conditions. However, the numerical method used to calculate the particle deposition has to be benchmarked before.

On the one hand Dr A. Dehbi, member of the LTH, has already carried out several benchmarking of turbulent particles dispersion models on wall-bounded geometries. The method then used is based on a CFD-Langevin-equation approach and it was applied for simple wall bounded geometries like straight pipe and 90° bend pipe. The results then obtained show good coherence with experimental data. However the geometry used is quite different from those of pebble beds. Therefore the method has to be benchmarked using geometries closer to a pebble bed.

On the other hand experiment of particles deposition on single and linear arrays of spheres experiments have been conducted. A pebble bed being a pile of spheres, benchmarking the model using these results will be a step further to obtain a numerical method that can be used on actual pebble bed geometry.

The investigation presented here consists on benchmarking this numerical method using particles deposition measurements on spheres. In a first part the theoretical aspects of the numerical method along with the experimental investigations are summarized. Then the two following parts present the application of the method; the second part presenting its CFD side and the third part presenting its particles tracking side. The benchmarking of the method is carried out in the third part.

1 Theory and background

This first part of the report gives some theoretical basis on particles diffusion modeling. It also concisely presents several other investigations linked to the study of particles deposition on spheres.

1.1 Particles tracking

In order to carry out numerical computations of particles deposition on collectors particles diffusion on a fluid has to be modeled. To do this it exist many different methods and models. This chapter gives basic information about those used for our study.

1.1.1 Particles Transport and Deposition mechanisms

Depending on the size of a particle and the nature of the flow, different mechanisms can be responsible for its transport and deposition.

Continuous phase influences motion of discrete particles through fluid forces such as:

- Drag: due to viscous and inertial effects of the fluid on particles, this force is always along direction of particle relative velocity and tends to make equal the particle velocity and the flow velocity. The drag force per unit mass may be expressed as :

  $$F_D = \mathrm{K_D}(u - u_p) = C_D.\frac{Re_p}{24}.\frac{18\mu}{\rho_p {d_p}^2}.(u - u_p)$$

  with:

  $$Re_p \equiv \frac{\rho_f d_p |u - u_p|}{\mu} = \text{ particles } relative\ Reynolds\ number$$
  $$C_D : Drag\ coeficient\ \ (its\ expression\ depends\ on\ the\ value\ of\ Re_p)$$
  $$\mu, \rho_f\ et\ u : fluid\ viscosity, density\ and\ velocity$$
  $$\rho_p\ , d_p\ et\ \ u_p : particle\ density, caracteristic\ length\ and\ velocity$$

  This force is always important.

- Gravity and Buoyancy: these two forces are along the gravitational acceleration and are in competition. The sum of the two can be expressed as (per unit mass):

  $$F_G = g\left(1 - \frac{\rho_f}{\rho_p}\right)$$

  Depend on the value of $\frac{\rho_f}{\rho_p}$ Gravity or Buoyancy will prevail.

- Lift: due to local velocity gradient or particle rotation, this force is always normal to particle relative velocity. This force is important for light particles ($\rho_p << \rho_f$) and secondary for heavy particles ($\rho_p >> \rho_f$).

- Brownian diffusion: due to the Brownian motion of particles in a fluid. Important only for small particles ($d_p < 0.1$ µm).

- Thermophoresis: due to temperature gradient in the fluid, this force tends to move aerosols toward the decreasing temperature. The thermophoresis force per unit mass may be expressed as :

  $$F_{th} = -D_{T,p}.\frac{1}{m_p T}\nabla T$$

  with:

  $$D_{T,p} : thermophoresis\ coeficient\ (depends\ on\ both\ fluid\ and\ particle)$$
  $$m_p : particle\ masse$$

When an important temperature gradient exists between the inlet air flow and the wall this mechanism can have a important influence on particle deposition rate.

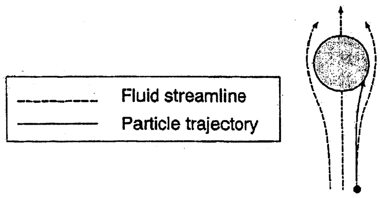
- Electrophoresis: due to presence of an electric field
- Photophoresis: due to intense light radiation
- Etc …

All transport mechanisms except for the drag force can bring a particle to contact a boundary of the fluid domain. Then, adhesives forces (e.g. Van der Waals force) tend to cause particles to adhere to the surface.

However, because of particle's inertia, it takes a certain amount of time for a particle to react to an acceleration of the fluid. In order to quantify this "reaction time", a temporal parameter depending on both particle and fluid has been defined. It is called the relaxation time and is defined as such:

$$\tau_p \equiv \frac{\rho_p {d_p}^2}{18\mu}$$

Thus, due to particle's inertia, an aerosol's trajectory may deviate from the fluid main streamline since it can be unable to follow the motion of an accelerating gaz. By following its own trajectory rather than the trajectory of a fluid passing around a solid object the aerosol can impact on the solid surface. This deposition mechanism is called **Inertial Impaction**.



In order to quantify this mechanism one uses the Stokes Number:

$$Stk \equiv \frac{\tau_p . u_\infty}{D_o} = \frac{Particle\ response\ distance}{caracteristique\ length}$$

with:

D_O : $caracteristique\ dimension\ of\ the\ obstacle$
u_∞ : $fluid\ main\ stream\ velocity$

Depending on the value of the Stokes Number, particle adjusts to flow and not impact on wall (Stk << 1), or mainly follows its own trajectory and impacts on wall (Stk << 1).

There exists another mechanism also due to particle inertia that can lead particle to deviate from a fluid main streamline. Turbulent eddies create fluctuating velocity component which are sometime normal to the main streamline. Depending on turbulence intensity and particles inertia, particles that only partially follow eddies motion are carried away from the main streamline. This phenomenon then affects particles concentration and doing so particles deposition. Moreover if a particle pass near a wall it can also be projected on it by turbulent fluctuations (see Figure 1).

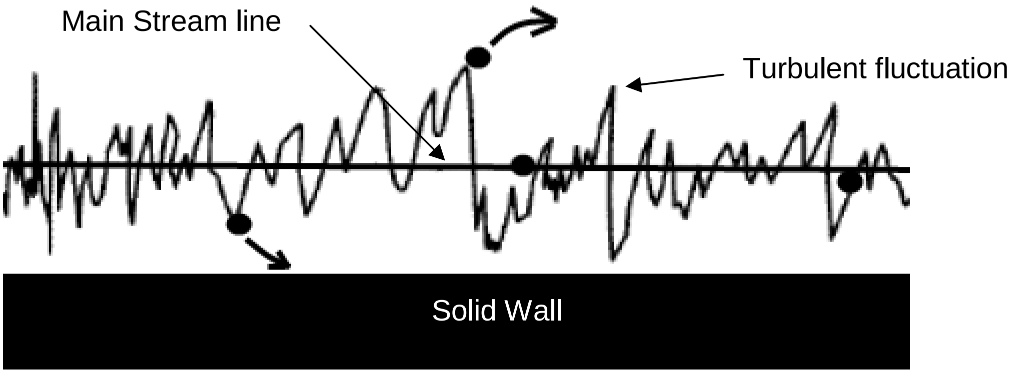


Figure 1 : Interaction particles/turbulent velocity fluctuation

Then two kind of inertial deposition mechanisms can be differentiated:

- → Inertial Impaction due to main velocity field and characterized by the Stokes number.
- → Turbulent-enhanced deposition due to fluctuating velocity.

That is why it is very important to accurately model turbulence and velocity fluctuations or particles deposition will sometime be highly underestimated.

Finally because of Particle Bounce or Re-entrainment particles impacting a wall have only a probability *h* to deposit. For solid collector and solid particles *h* can fall to only a few percent.

1.1.2 Particles tracking methods and equations

There are two main families of methods to treat particle transport in fluid flows: Eulerean and Lagrangian.

— In the Eulerean or “two-fluid” approach, the particles are regarded as a continuous phase for which the averaged conservation equations (continuity, momentum and energy) are solved in similar fashion to the carrier gas flow. The Eulerean approach is particularly suitable for denser suspensions when particle–particle interactions are important and the particle feedback on the flow is too large to ignore.

— In the second approach, called Lagrangian, the particles are treated as a discrete phase made of particles which are dispersed in the continuous phase. The particle volume loading is usually assumed negligible, so that particles have no feedback effect on the carrier gas and particle–particle interactions are neglected. In the Lagrangian framework, the controlling phenomena for particle dispersion in the field are assessed using a rigorous treatment of the forces acting on the particle. In general, the detailed flow field is computed first, then a representatively large number of particles are injected in the field, and their trajectories determined by following individual particles until they are removed from the gas stream or leave the computational domain. Particle motion is extracted from the time integration of Newton’s second law, in which all the relevant forces can be incorporated (drag, gravity, lift, thermophoretic force, etc.). The Lagrangian approach is computationally intensive, because it entails tracking a large number of particles until stationary statistics are achieved. On the other hand, the results of Lagrangian particle tracking are physically easier to interpret. Therefore, in the following investigation, the Lagrangian methodology is used, along with the assumption that the dispersed phase is dilute enough not to affect the continuous flow field.

The methods used here are Lagrangian ones. Then the equations used for these methods are detailed below.

When applying the Newtown's second law to a particle we obtain the following equation (the fluid velocity *u* has been solved previously independently of any particles tracking):

$$\frac{du_p}{dt} = K_D.\left(u - u_p\right) + \mathrm{F_G} + \mathrm{F_{th}} + \mathrm{Lift} + \cdots$$

The trajectory x(x1,x2,x3, t) of the particle is obtained by integration of the following velocity vector equation with respect to time:

$$\frac{dx}{dt} = u_p$$

In laminar flows only the averaged velocity field is influencing particles motion and the previous expressions are sufficient to compute the trajectory of individual particles whatever the method used to solve the flow (RANS, LES or DNS). As particles trajectory is deterministic few trajectory computation are needed to obtain the mean dispersion statistics.

In turbulent flows, random velocity fluctuations are also influencing particles motion. And when turbulent fluctuations exist in the fluid flow, the computation of particle trajectory is no longer deterministic and the particle tracking problem becomes more complicated to handle. To determine the mean dispersion statistics of particles it is necessary to perform many trajectory computations to obtain correct averaged results.

If the flow has been solved with DNS or LES velocity fluctuations are already included into the velocity field. So particles trajectory can be directly computed with no need of further modeling. However, DNS and LES are still very time-consuming process and not fitted for complex 3D geometry.

While using RANS method only the time averaged velocity field is available and turbulence is represented through variables like turbulent kinetic energy, turbulence dissipation rate or Reynolds Stresses components. Then one needs to model the effects of velocity fluctuations on particles.

That is why stochastic models of the fluid velocity fluctuations have been created in order to model the effect of turbulence on Largangian particles. For that one uses a Random Walk model consisting of a large number of independent steps with statistic components in each step. Random Walk models are treatments in which particles are made to interact with the instantaneous velocity field u such as:

$$u(t) = \bar{u} + u'(t)$$

with:

$\bar{u}$: mean velocity
$u'(t)$: fluctuating velocity

Two different kind of Random Walk model are presented here: the Discrete Random Walk Model (CRW) which is implemented in Fluent, and the Continuous Random Walk Model (CRW). These two models have been benchmarked many times by several people and they are described here as in [2] & [3] (A. Dehbi).

In these two models the mean flow is previously solved either by using a steady CFD-RANS method or by averaging an unsteady solution obtain by URANS, DES or LES. Then the Random Walk model is applied in order to model the action of the velocity field on particles.

- DRW model

Here the turbulent dispersion of particles is modeled as a succession of interactions between a particle and eddies which have finite lengths and lifetimes. It is assumed that at time t_0, a particle with velocity u_p is captured by an eddy which moves with a velocity composed of the mean fluid velocity, augmented by a random "instantaneous" component which is piecewise constant in time. When the lifetime of the eddy is over or the particle crosses the eddy, another interaction is generated with a different eddy, and so forth. The eddy has the following length and lifetime:

$$L_e = C_\mu^{\frac{3}{4}}.\frac{k^{\frac{3}{2}}}{\varepsilon}$$
$$\tau_e = C_L.\frac{k}{\varepsilon}$$

with:

$C_\mu \text{ and } C_L : \text{constants dependent on the model of turbulence used}$
$k : \text{turbulent kinetic energy (obtained in the RANS modeling)}$
$\varepsilon : \text{dissipation rate of kinetic energy (obtained in the RANS modeling)}$

Then the value of the turbulent gas velocity which prevails during the eddy lifetime is randomly drawn from a Gaussian distribution. Hence, in component notation, one has:

$$u_i' = \lambda_i.\sqrt{\overline{u_i'^2}} \quad avec \quad i = 1, 2 \ ou \ 3$$

with:

$\lambda_i : \text{random numbers with zero mean and unit standard deviation.}$

In the bulk of the flow, where the turbulence is assumed isotropic, the rms values of the three components of instantaneous velocity are obtain from the relationship:

$$\sqrt{\overline{u_1'^2}} = \sqrt{\overline{u_2'^2}} = \sqrt{\overline{u_3'^2}} = \sqrt{\frac{2k}{3}}$$

However, when used in the boundary layer the previous expression introduce a large over-prediction for the wall normal component u_2'. That is why when the particle is inside the boundary layer ($y^+ < 100$) the rms values of instantaneous velocity and turbulence dissipation rate are modified to account for the strong anisotropic nature of turbulence. For that one uses correlations extracted from DNS results:

$$u_1'^+ = \frac{\sqrt{\overline{u_1'^2}}}{u^*} = \frac{0.40y^+}{1 + 0.0239(y^+)^{1.496}}$$
$$u_2'^+ = \frac{\sqrt{\overline{u_2'^2}}}{u^*} = \frac{0.0116(y^+)^2}{1 + 0.203y^+ + 0.00140(y^+)^{2.421}}$$
$$u_3'^+ = \frac{\sqrt{\overline{u_3'^2}}}{u^*} = \frac{0.19y^+}{1 + 0.0361(y^+)^{1.322}}$$
$$\varepsilon^+ = \frac{\varepsilon}{u^{*4}/\upsilon} = \frac{1}{4.529 + 0.0116(y^+)^{1.75} + 0.768(y^+)^{0.5}}$$

with:

$$u^* = \sqrt{\frac{\tau_w}{\rho_f}} : \text{ friction velocity}$$

$$\upsilon : \text{fluid kinematic viscosity}$$

Despite being quite cheap in CPU time and giving some good results the DRW method suffer from fundamental shortcoming:

— Particle velocity jumps at end of eddy lifetime (infinite acceleration)

— Non-physical accumulation of small particles close to walls, so called "spurious drift", which leads to non-physical deposition of small inertia particles on walls.

- <u>CRW model:</u>

The CRW model have been created to offer a more physical way of modeling the fluctuating velocity, and thus go past the shortcoming of the DRW model.

One of the most common ways to describe fluid velocity fluctuations in a continuous way is through the Langevin equation. In this equation the change in the fluid velocity field with time is assumed to be comprised of a damping term which is proportional to velocity, and a random forcing term that has zero mean. Thus the Langevin equation is a stochastic differential equation which uses Markov chains to specify a possible increment du_i in the fluid velocity fluctuation during a time dt:

$$du_i' = -u_i'(t)\frac{dt}{\tau_i} + \sigma_i\sqrt{\frac{2}{\tau_i}}.d\xi_i$$

with:

$$\tau_i : \text{timescale caracteristic of the turbulence}$$

$$\sigma_i = \sqrt{\overline{u_i'^2}} \;:\; \text{rms of flucuating velocity}$$

$$d\xi_i : \text{random numbers with zero mean and variance } dt$$

The Langevin equation was extensively used to model homogeneous turbulence where the rms values and timescales are position independent. In wall-bounded flow, however, turbulence is strongly inhomogeneous and anisotropic in the boundary layer, which implies some modification of the Langevin equation is in order.

First, one must take the impact of turbulence inhomogeneities into account. Without this correction tracer-like particles will diffuse in a non-physical way and induce errors as high as 550 % in simple flows. The inclusion of the drift acceleration into the Lagrangian equation dramatically decreases these errors. With $a_i = u_j\frac{\partial u_i}{\partial x_j}$ the instantaneous acceleration of a fluid particle, the drift acceleration is defined as followed:

$$\overline{a_i} = a_{i,mean} + a_{i,drift} = \overline{u_j}\frac{\partial \overline{u_i}}{\partial x_j} + \overline{u_j'\frac{\partial u_i'}{\partial x_j}}$$

The drift acceleration gives rise then to a drift velocity that one needs to add in the Langevin equation to take into account turbulence inhomogeneities:

$$\delta u_i = \overline{u_j'\frac{\partial u_i'}{\partial x_j}}dt = \frac{\partial \overline{u_j'u_i'}}{\partial x_j}dt$$

To arrive at the second equality, it is necessary to assume a divergence-free fluctuating velocity field, which is reasonable for the incompressible flows addressed in this investigation.

However, the previous expression of the drift velocity is valid for a fluid particles and thus for tracer-like particles only. For inertial particles a correction is in order. One can shows that the drift correction for an inertial particle can be obtained from the drift correction of a fluid particle through a multiplicative factor as follow:

$$\delta u_i = \frac{\partial \overline{u_j' u_i'}}{\partial x_j} . \left(\frac{1}{1 + Stk}\right) . dt$$

with:

$Stk = \frac{\tau_p}{\tau_L}$: *particles Stokes number*

τ_L : Lagrangian time scale (to be specified)

τ_p : Particle relaxation time

Thus the Langevin equation can be written as follows:

$$du_i' = -u_i' . \frac{dt}{\tau_i} + \sigma_i \sqrt{\frac{2}{\tau_i}} . d\xi_i + \frac{\partial \overline{u_j' u_i'}}{\partial x_j} . \left(\frac{1}{1 + Stk}\right) . dt$$

Secondly, the Langevin equation is normalized in order to better account of both the inhomogeneous and anisotropic nature of the turbulence in the boundary layer:

$$d\left(\frac{u_i'}{\sigma_i}\right) = -\left(\frac{u_i'}{\sigma_i}\right) . \frac{dt}{\tau_i} + \sqrt{\frac{2}{\tau_i}} . d\xi_i + \frac{\partial \left(\frac{\overline{u_j' u_i'}}{\sigma_i}\right)}{\partial x_j} . \left(\frac{1}{1 + Stk}\right) . dt$$

Finally a distinction is made between turbulence in the bulk flow and in the boundary layer:

→ In the bulk flow the turbulence is considered isotropic so :

$$\sigma_1 = \sigma_2 = \sigma_3 = \sigma = \sqrt{\frac{2k}{3}}$$

After simplifications the Langevin equation became:

$$d\left(\frac{u_i'}{\sigma}\right) = -\left(\frac{u_i'}{\sigma}\right) . \frac{dt}{\tau_L} + \sqrt{\frac{2}{\tau_L}} . d\xi_i + \frac{1}{3\sigma} \frac{\partial k}{\partial x_j} . \left(\frac{1}{1 + Stk}\right) . dt$$

with:

$$\tau_L = \frac{2}{C_0} \frac{k}{\varepsilon}$$