This is document is incomplete and in draft form.

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The purpose of this document is to describe the PFC fluid flow options.

1 Coarse Grid Schemes

Two implementations of volume averaged coupling between discrete particles and a continuous fluid phase are available in PFC3D. The "Fixed Coarse-Grid Fluid Scheme" was introduced in PFC 3.1 and will be referred to as CGFS in this document. The CCFD Add-on is being introduced in PFC3D 4.0 and will be referred to as CCFD in this document.

Both of these "coarse grid schemes" use similar assumptions about how the discrete particles and the fluid interact. In both the CGFS and CCFD, the Navier-Stokes equation formulated with a porosity term and an additional body force term to account for the presence of particles in the fluid,

$$\rho_f \frac{\partial \epsilon \vec{v}}{\partial t} + \rho_f \vec{v} \cdot \nabla(\epsilon \vec{v}) = -\epsilon \nabla p + \mu \nabla^2 (\epsilon \vec{v}) + \vec{f_b} \tag{1}$$

and expressing the conservation of volume as,

$$\frac{\partial \epsilon}{\partial t} + \nabla \cdot (\epsilon \vec{v}) = 0 \tag{2}$$

where ρ_f is the density of the fluid, ϵ is porosity, $\vec{v}$ is the fluid velocity, p is the fluid pressure, μ is the dynamic viscosity of the fluid and $\vec{f_b}$ is a body force per unit volume.

The domain over which the problem is to be solved is discretized into a set of elements[1]. The porosity and body force in these fluid elements are determined by PFC. The fluid velocity and fluid pressure are determined, in the fluid code, by solving the equations of motion of the fluid using a finite volume method.

The comparison between these codes consists of brief theoretical descriptions of each code and a comparison of results on idealized examples.

1.1 CGFS: "Fixed Coarse-Grid Fluid Scheme"

This code is available in 2D and 3D. It is part of the main PFC executable and does not require any additional programs. The geometry of the problem domain is limited to rectangular shapes with regular hexahedral elements. The fluid boundary conditions can be applied to the faces of the rectangular domain.

This option also support thermal coupling between the fluid and the discrete particles (REFERENCE).

[1] The length scale of the elements must be such that several particles can fit inside one element. This has the consequence that the length scale of fluid structures to be modeled must be larger than the particle length scale.

1.1.1 Theory

The early work in this type of particle/fluid interaction was done by Professor Tsuji and others at Osaka University (REFERENCE). A similar scheme is implemented as the CGFS in PFC (REFERENCE).

The drag force applied to the fluid in each fluid element is calculated as,

$$\vec{f_b} = \beta \vec{U} \tag{3}$$

where, $\vec{f_b}$ is the drag force per unit volume, β is a coefficient and $\vec{U}$ is the average relative velocity between the particles and the fluid defined as,

$$\vec{U} = \bar{\vec{u}} - \vec{v} \tag{4}$$

where $\vec{v}$ is the fluid velocity and $\bar{\vec{u}}$ is the average particle velocity of all particles in a given fluid element defined as,

$$\bar{\vec{u}} = \frac{1}{N} \sum_j \vec{u}^j \tag{5}$$

where the sum is over all particles occurring in a fluid element.

Following Tsuji the coefficient β is calculated in one of two ways depending on the porosity of the fluid element. For low values of porosity ($\epsilon < 0.8$) the Ergun relation is used (REFERENCE). The relation is derived from observations of pressure drop in flow through porous materials.

$$\beta = \frac{(1-\epsilon)}{\bar{d}^2 \epsilon^2} \left(150(1-\epsilon)\mu + 1.75 \rho_f \bar{d} |\vec{U}| \right) \qquad \epsilon < 0.8 \tag{6}$$

μ is the dynamic viscosity of the fluid, ρ_f is the density of the fluid, ϵ is the porosity and $\bar{d}$ is the average diameter of the particles occurring in the element

$$\bar{d} = \frac{1}{N} \sum_j d^j \tag{7}$$

where the sum is over all particles in a given fluid element.

In (6) the first term in the parenthesis on the right hand side is dominant at low Reynolds numbers and at low porosity. The form of this term can be compared to the Kozney-Carman relation for porous flow (REFERENCE). The second term becomes dominate at higher Reynolds numbers where turbulent effects occur.

For higher values of porosity ($\epsilon \geq 0.8$) β is derived from the corrected nonlinear drag force exerted on a spherical particle by a fluid (REFERENCE)

$$\beta = \frac{4}{3} C_d \frac{|\vec{U}| \rho_f (1-\epsilon)}{\bar{d} \epsilon^{1.7}} \qquad \epsilon \geq 0.8 \tag{8}$$

where C_d is a turbulent drag coefficient defined in terms of the particle Reynolds number

$$C_d = \begin{cases} \frac{24(1+0.15 Re_p^{0.687})}{Re_p} & Re_p < 1000 \\ 0.44 & Re_p > 1000 \end{cases} \tag{9}$$

where

$$Re_p = \frac{|\vec{U}|\rho_f \epsilon \bar{d}}{\mu}. \tag{10}$$

The equations above give the body force experienced by the fluid as a result of the moving particles. A force equal and opposite is distributed to the discrete particles in each fluid element. The drag force applied to individual discrete particles is,

$$\vec{f}_{drag} = \frac{4}{3}\pi r^3 \frac{\vec{f}_b}{(1-\epsilon)} \tag{11}$$

where r is the particle radius and $\vec{f}_b$ is the drag force per unit volume in the fluid element the particle occupies. The total force exerted by the fluid on the particle is the sum of the drag force and the buoyancy force.

$$\vec{f}_{fluid} = \vec{f}_{drag} + \frac{4}{3}\pi r^3 \rho_f \vec{g} \tag{12}$$

1.2 CCFD Add-on: Coupled Computational Fluid Dynamics

This Add-on is available for PFC3D only. The package includes a third party pre/post-processor called GiD and flow solver called CCFD. Unstructured tetrahedral and mapped hexahedral elements can be used and there is no limit on the geometry of the problem domain.

1.2.1 Theory

The drag force calculation is done differently in CCFD. To calculate the total drag force in a fluid element the drag force exerted on each particle is calculated individually and is summed.

The drag force on a particle $\vec{f}_{drag}$ is defined as:

$$\vec{f}_{drag} = \vec{f}_0 \epsilon^{-\chi}. \tag{13}$$

$\vec{f}_0$ is the drag force on a single particle and ϵ is the porosity of the fluid element in which the particle resides. The $\epsilon^{-\chi}$ term is an empirical factor to account for the local porosity. This correction term makes the force applicable to both high- and low-porosity systems and for a large range of Reynolds numbers (Di Felice 1994, Xu and Yu 1997). As above, the total force exerted by the fluid on the particle is the sum of the drag force and the buoyancy force.

$$\vec{f}_{fluid} = \vec{f}_{drag} + \frac{4}{3}\pi r^3 \rho_f \vec{g} \tag{14}$$

The single particle force is defined as,

$$\vec{f}_0 = \left(\frac{1}{2} C_d \rho_f \pi r^2 |\vec{u} - \vec{v}|(\vec{u} - \vec{v})\right), \tag{15}$$

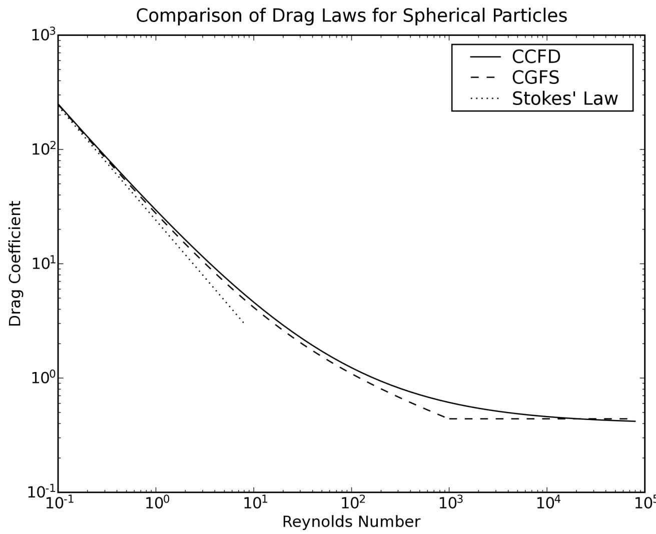

Figure 1: Comparison of Stokes Law with the drag laws used by the CGFS and CCFD.

where C_d is a drag coefficient, ρ_f is the fluid density, r is the particle radius, $\vec{v}$ is the fluid velocity and $\vec{u}$ is the particle velocity. The drag coefficient is defined as,

$$C_d = \left(0.63 + \frac{4.8}{\sqrt{Re_p}}\right)^2, \tag{16}$$

where Re_p is the particle Reynolds number. The empirical coefficient χ is defined as,

$$\chi = 3.7 - 0.65 \exp\left(-\frac{(1.5 - \log_{10} Re_p)^2}{2}\right) \tag{17}$$

The particle Reynolds number is,

$$Re_p = \frac{2\rho_f r|\vec{u} - \vec{v}|}{\mu_f} \tag{18}$$

where μ_f is the dynamic viscosity of the fluid.

The body force per unit volume exerted on the fluid is

$$\vec{f_b} = \frac{\sum_j \vec{f^j}_{drag}}{V} \tag{19}$$

where V is the volume of the fluid element.

2 Example models

2.1 Falling ball

In this example we consider a single particle settling under gravity in a fluid which is initially at rest. The equation of motion for a settling particle is

$$\frac{4}{3}\pi r^3 \rho_p \frac{du_z}{dt} = \frac{4}{3}\pi r^3 \left(\rho_p - \rho_f\right) g - \frac{1}{2}\pi r^2 \rho_f C_d u_z^2 \tag{20}$$

Where u_z is the vertical velocity. When the particles reaches terminal velocity $\frac{du_z}{dt}$ becomes zero,

$$\frac{1}{2}\pi r^2 \rho_f C_d u_z^2 = \frac{4}{3}\pi r^3 \left(\rho_p - \rho_f\right) g \tag{21}$$

The CGFS and CCFD use different model assumptions for the drag on a spherical particle is ((9) and (16)). In both cases, substituting the definition of C_d results in an expression which is non-linear and can not be solved directly. A numerical solution is possible using a Newton-Raphson method (see ccfd-newton-raphson.dat and cgfs-newton-raphson.dat).

2.1.1 Case 1: Particle falling at low Reynolds number

A glass sphere 1cm in diameter settling in Glycerol. The density and dynamic viscosity of the fluid are 1260 km^{-3} and 1.5 Pa·s respectively and the particle density is 2500 kgm^{-3}. The fluid domain is a cube of dimension 1m, the domain is discretized into a mesh of 9 by 9 by 9 hexahedral elements. Equation 23 (Stokes law) gives a velocity of -4.50e-2ms^{-1} for this case. This velocity gives a Reynolds number of 0.38.

For small Reynolds numbers it has been shown that the drag coefficient can be defined exactly (REFERENCE)

$$C_d = \frac{24}{Re_p} \tag{22}$$

Assuming that the falling particle does not accelerate the fluid allows for a closed form solution to (21) known as Stokes Law,

$$u_z = -\frac{2}{9}\frac{r^2(\rho_p - \rho_f)g}{\mu_f} \quad for \quad Re_p \ll 1 \tag{23}$$

Figure 2 shows the particle velocity as a function of time as calculated by the CGFS and CCFD. The dashed lines show the model solutions for the CGFS and CCFD and the solid black line shows the velocity predicted by Stokes law. In both the CGFS and CCFD, the particle accelerates quickly to the terminal velocity and after 0.06 seconds the particle continues to accelerate slowly as the fluid around the particle is accelerated. Both codes give comparable results to Stokes law but they are not identical as a result of the different particle drag laws. Figure 1 compares Stokes law with the drag models used in the CGFS

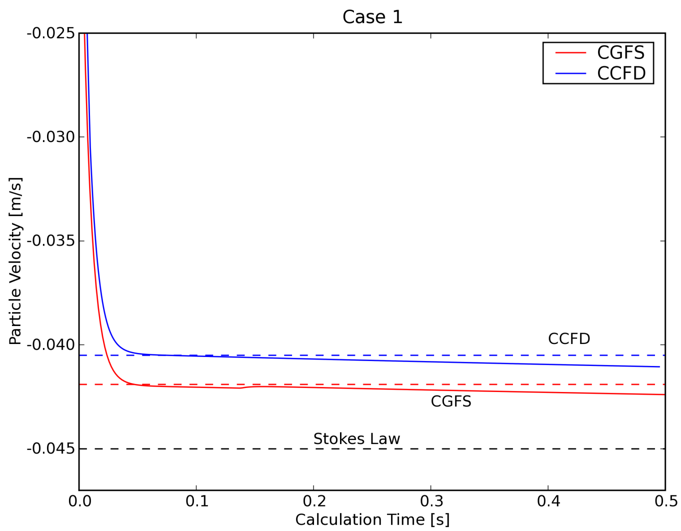

Figure 2: Plot of results for Case 1.

and CCFD. As the Reynolds number tends to zero all three functions converge. At higher Reynolds numbers there is some divergence. The following table summarizes the results.

Case 1	Model solution	Coupled Solution at 0.5s
Stokes Law	-4.50e-2ms^{-1}	N/A
CGFS (model)	-4.19e-2ms^{-1}	-4.24e-2ms^{-1}
CCFD (model)	-4.05e-2ms^{-1}	-4.11e-1ms^{-1}

2.1.2 Case 2: Particle falling at high Reynolds number

A particle 1mm in diameter with a density of 2650kgm^{-3} settling in still water. The density and viscosity of water are 998.23 kgm^{-3} and 1.004e-3 Pa·s respectively. The same fluid domain and mesh are used. At higher Reynolds numbers Stokes Law (23) is no longer valid and no other closed form solution in available.

Figure 2 shows the particle velocity as a function of time as calculated by the CGFS and CCFD. The dashed lines show the model solutions. The agreement with model solutions in good in both cases. The table below summarizes the results.

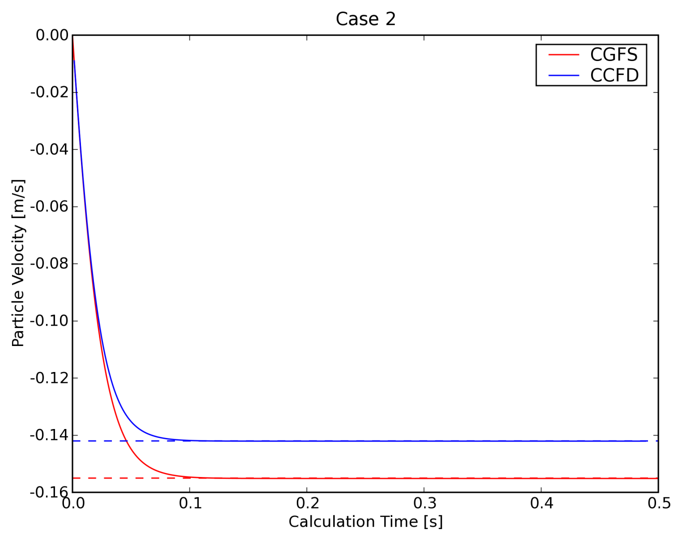

Figure 3: Plot of results for Case 2.

Case 2	Model solution	Coupled solution at 0.5s
Stokes Law	N/A	N/A
CGFS (model)	-1.55e-1ms^{-1}	-1.55e-1ms^{-1}
CCFD (model)	-1.42e-2ms^{-1}	-1.42e-1ms^{-1}

2.2 Saturated Porous Flow

The motion of fluid in a saturated porous medium is described by Darcy's Law,

$$Q = -\frac{AK}{\mu_f}\nabla p \tag{24}$$

where Q is the volumetric flow rate in m$^3 s^{-1}$, K is permeability with units m^2, A is a cross sectional area, μ_f is the dynamic viscosity of the fluid and ∇p is the fluid pressure gradient. The permeability K is a tensor property of the porous medium independent of the fluid. Permeability is often assumed to be isotropic, and is generally proportional to the porosity and the grain size squared.

Several theoretical formulations describe the macroscopic permeability of materials with regular flow pathways. The Kozeny-Carman relation is widely used to estimate the permeability of a porous material in terms of the grain size and porosity,

$$K = B\frac{\epsilon^3}{(1-\epsilon)^2}d^2 \tag{25}$$

where B is a geometric factor taken as 1/180 ϵ is porosity, and d is the diameter of the particles.

2.2.1 Case 3: Flow in a regular fixed porous medium

Water flow in a regular saturated porous medium under a fixed pressure gradient. A repeating arrangement of particles each with radius 1.25e-3m is created in a rectangle with a length of 0.1m and height and width of 0.05m. There are 16,000 particles total and the particles are fixed in place. The porosity is 0.476 A pressure gradient of 1.0e2 Pa is imposed across the length and the volumetric flow rate is observed.

For this idealized case, an approximate solution to the Navier-Stokes equation (1) can be found. The terms on the left-hand side of (1) become zero for a steady flow. The steady system is a balance between the three terms on the right hand side: $-\epsilon\nabla p$ is the applied pressure gradient, $\mu\nabla^2(\epsilon\vec{v})$ is the momentum loss due to viscosity, and $\vec{f_b}$ is a body force which describes the drag force exerted by the particles on the fluid.

In the general case of fully saturated porous flow, the viscous term is large and balances the applied pressure gradient. In the present model (the CGFS and CCFD), the viscous stresses applied by the surface of each particle to the fluid are not calculated directly. (The viscous stresses on the grain surfaces is the micro scale mechanism of permeability.) In the coarse grid schemes, model assumptions are made about the force exerted on spherical particles due to fluid movement. This drag force is then applied to the fluid as a volume averaged body force. This assumption has the consequence that the viscous term of (1) only accounts for the viscous momentum loss due to macroscopic fluid velocity gradient and interaction with "no slip" fluid domain boundaries.

In Case 3, the velocity field is uniform and the viscous losses associated with the domain boundaries are small relative to the pressure gradient and the particle drag force. Assuming the viscous term is small, (1) can be reduced to

$$\epsilon\nabla p = \vec{f_b} \tag{26}$$

In the CGFS $\vec{f_b}$ is defined in (3) with this substitution (26) has the form,

$$\epsilon\nabla p = \beta|\vec{u} - \vec{v}| \tag{27}$$

This equation has a solution for fluid velocity in the following expression (see cgfs-case3.wxm),

$$v = \frac{\sqrt{(1-\epsilon)\,4\,\bar{d}^3\,\epsilon^3\,|\nabla p|\,\rho_f\,C_2 + (\epsilon-1)^4\,\mu^2\,{C_1}^2} - C_1\mu(\epsilon-1)^2}{2\,\bar{d}\,(1-\epsilon)\,\rho_f\,C_2} \tag{28}$$

where C_1 and C_2 are constants with values 150.0 and 1.75. In CCFD $\vec{f_b}$ is defined in (19) with this substitution (26) has the form,

$$\epsilon\nabla p = \frac{N_p\vec{f_0}\epsilon^{-\chi}}{V} \tag{29}$$

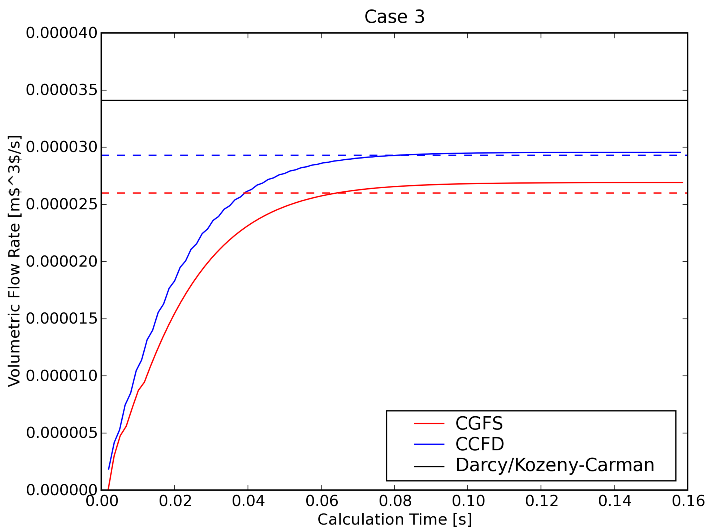

Figure 4: Plot of results for Case 3.

where N_p is the number of particles occurring in each fluid element (4^3 in this case). A numerical solution for fluid velocity can be obtained from this equation (see ccfd-case3.wxm).

The following table compares the fluid velocities predicted for Case 3. The table compares the Darcy/Kozeny-Carman model, the model solutions to (26) for the CGFS and CCFD, and the coupled numerical results from the CGFS and CCFD. Note that these flow rates show the steady state and the time dependent behavior of the velocity is a result of the linear relaxation.

Case 3	Model solution	Coupled solution
Darcy / Kozeny-Carman	Q = 3.41e-5 m$^3 s^{-1}$ v = 1.36e-2 ms^{-1}	N/A N/A
CGFS	Q = 2.60e-5 m$^3 s^{-1}$ v = 1.04e-2 ms^{-1}	Q = 2.69e-5 m$^3 s^{-1}$ v = 1.08e-2 ms^{-1}
CCFD	Q = 2.93e-5 m$^3 s^{-1}$ v = 1.17e-2 ms^{-1}	Q = 2.95e-5 m$^3 s^{-1}$ v = 1.18e-2 ms^{-1}

Figure 4 shows the volumetric flow rates as a function of time for both models.

2.2.2 Case 4: Flow in a random porous material

The Itasca FISH TANK is used to generate a rectangular granular specimen of height 63.2e-3m and length and width of 31.7e-3m. The average particle radius is 7.0e-4m and there are 12,251 particles total. The average porosity is 0.378. A pressure gradient of 2.0e3 Pa is applied across the specimen and the volumetric flow rate is observed.

Case 4	Volumetric flow rate Q
Darcy / Kozeny-Carman	Q = 7.92e-5 m$^3 s^{-1}$
CGFS	Q = 4.17e-5 m$^3 s^{-1}$
CCFD	Q = 4.15e-5 m$^3 s^{-1}$

2.3 Fluidized Bed

In a fluidized bed the weight of a particle is balanced by the drag force and buoyancy force exerted by the fluid on that particle. The drag force a particle experiences is a function of the local porosity and other terms. These ideas can be used to seek steady-state solutions of bed height which can be compared to the results of a coupled calculation.

2.3.1 Steady Fluidization Solutions for the CGFS

For the drag model used in the CGFS the balance of forces acting on a particle can be written as,

$$\frac{4}{3}\pi r^3(\rho_p - \rho_f)\vec{g} = \frac{4}{3}\pi r^3 \frac{\beta|\vec{U}|}{1-\epsilon} \tag{30}$$

In most cases relevant to fluidization the porosity, ϵ will be less that 0.8 so we use Ergun's Law for the definition of β. When the system reaches an idealized steady state the porosity is constant, the particles are not moving and the fluid velocity does not deviate from the vertical direction. In the steady state the relative velocity $\vec{U}$ can be replaced with the fluid velocity, $\vec{v}$. With these substitutions the steady-state equation becomes,

$$(\rho_p - \rho_f)\vec{g} = \frac{v}{\bar{d}^2\epsilon^2}\left(150(1-\epsilon)\mu + 1.75\rho_f\bar{d}|\vec{v}|\right) \tag{31}$$

Assuming the fluidization is uniform only the porosity, ϵ changes as the bed height increases. Solving for ϵ in (31) gives (see cgfs-case5.wxm),

$$\epsilon = \frac{\sqrt{\left(4\bar{d}^3\rho_f|\vec{v}|^2C_2 + 4\bar{d}^2\mu|\vec{v}|C_1\right)(\rho_p-\rho_f)|\vec{g}| + \mu^2|\vec{v}|^2C_1^2} - \mu|\vec{v}|C_1}{2\bar{d}^2(\rho_p-\rho_f)|\vec{g}|} \tag{32}$$

where C_1 is 150 and C_2 is 1.75. Once the porosity is known the height of the bed can be calculated as

$$h = \frac{N_p \frac{4}{3}\pi r^3}{(1-\epsilon)lw} \tag{33}$$

where h is the steady height of the bed, l and w are the length and width of the container and N_p is the number of particles in the bed.

2.3.2 Steady Fluidization Solutions for CCFD

For the drag assumptions used in CCFD the balance between drag force and bouyancy can be expressed as,

$$\frac{4}{3}\pi r^3(\rho_p - \rho_f)\vec{g} = \vec{f_0}\epsilon^{-\chi} \tag{34}$$

where $\vec{f_0}$ and χ are defined in (15) and (17) respectively. This equation can be solved directly for porosity, ϵ,

$$\epsilon = \left(\frac{\frac{4}{3}\pi r^3(\rho_p - \rho_f)\vec{g}}{\vec{f_0}}\right)^{\frac{-1}{\chi}} \tag{35}$$

As above the steady-state bed height can be calculated once the porosity is known.

2.3.3 Case 5: Fluidized bed

Water is pumped at $0.04ms^{-1}$ through a rectangular box containing a granular material causing the granular material to fluidize. The box has a height of 0.1m and a length and width of 9.5174e-3m. 2000 particles are present in the container. The radius of the particles is 3.675e-4m and the density of the particles is 2465 kgm^3. The calculation is run for two seconds.

For these parameters the results of the steady model solutions are given in the table below

Case 5	Steady Porosity	Steady Bed Height
CGFS	0.703	1.55e-2m
CCFD	0.643	1.30e-2m

The top plot in figure 5 shows the calculated bed heights as a function of time along with the steady-state solutions for both the CGFS and for CCFD.

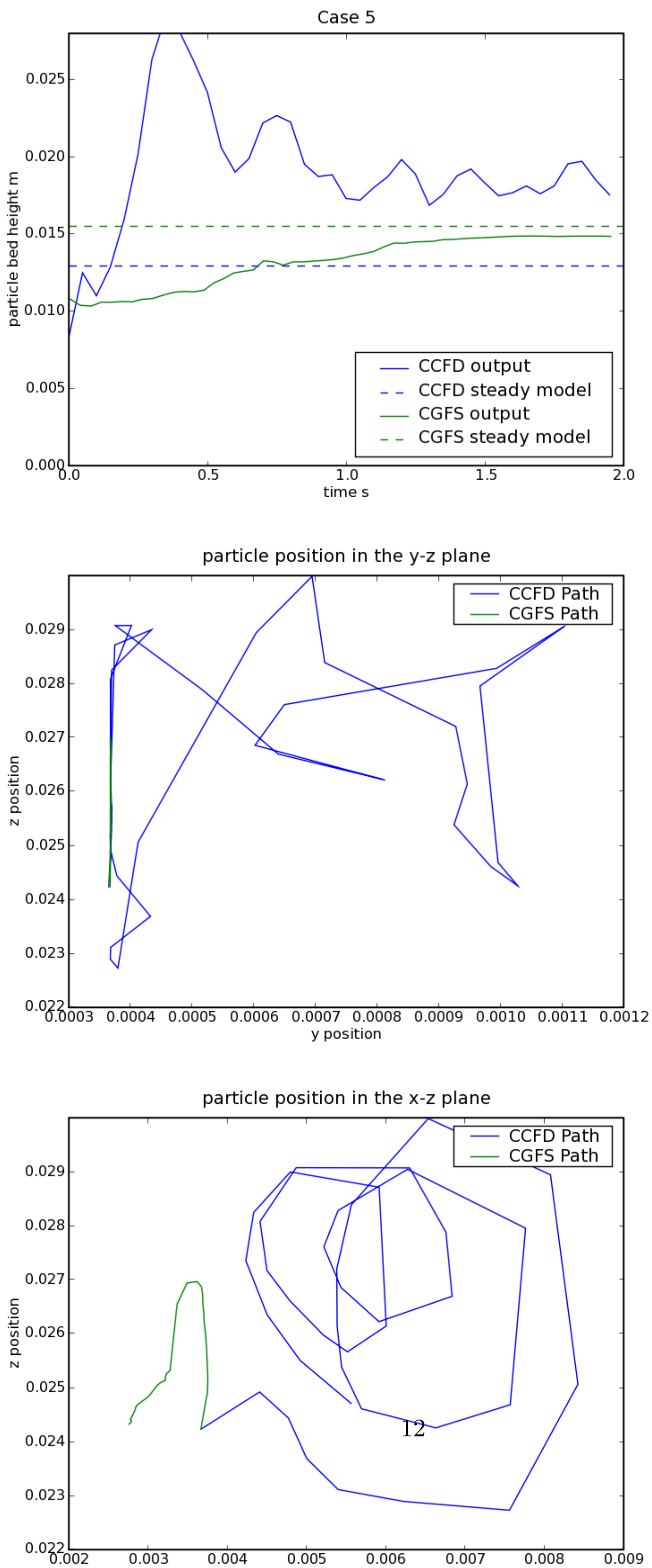

Figure 5: Plot of results for Case 5.