

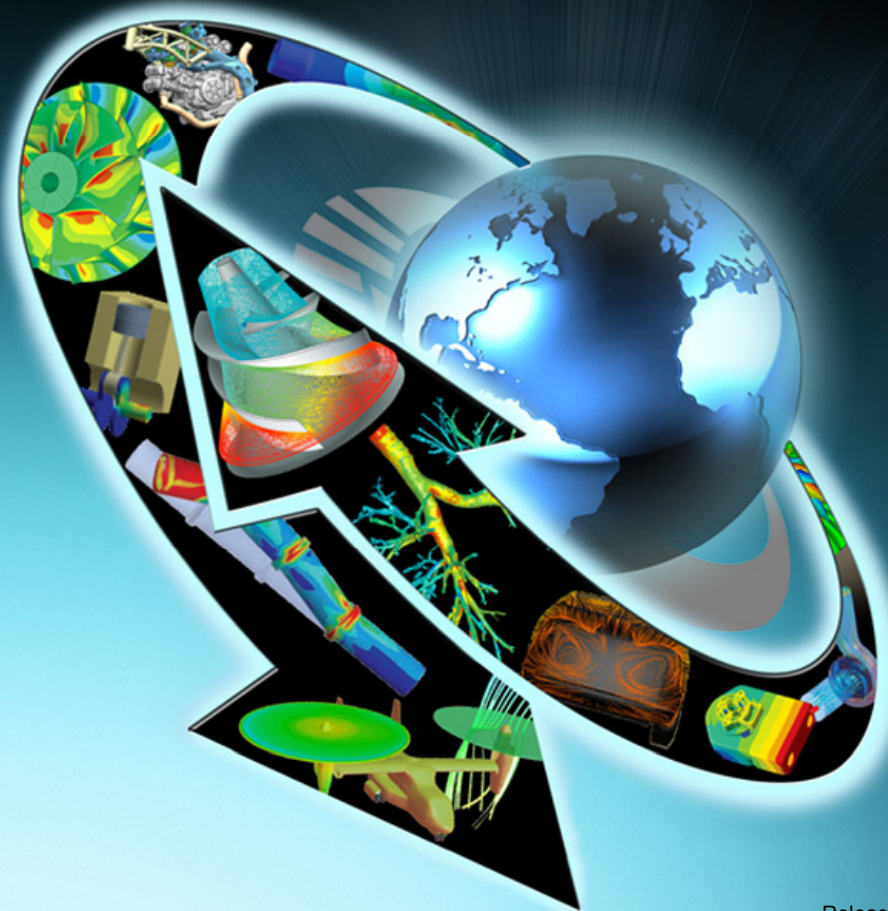


Customer Training Material

Workshop 6

Using the Discrete Phase Model (DPM)

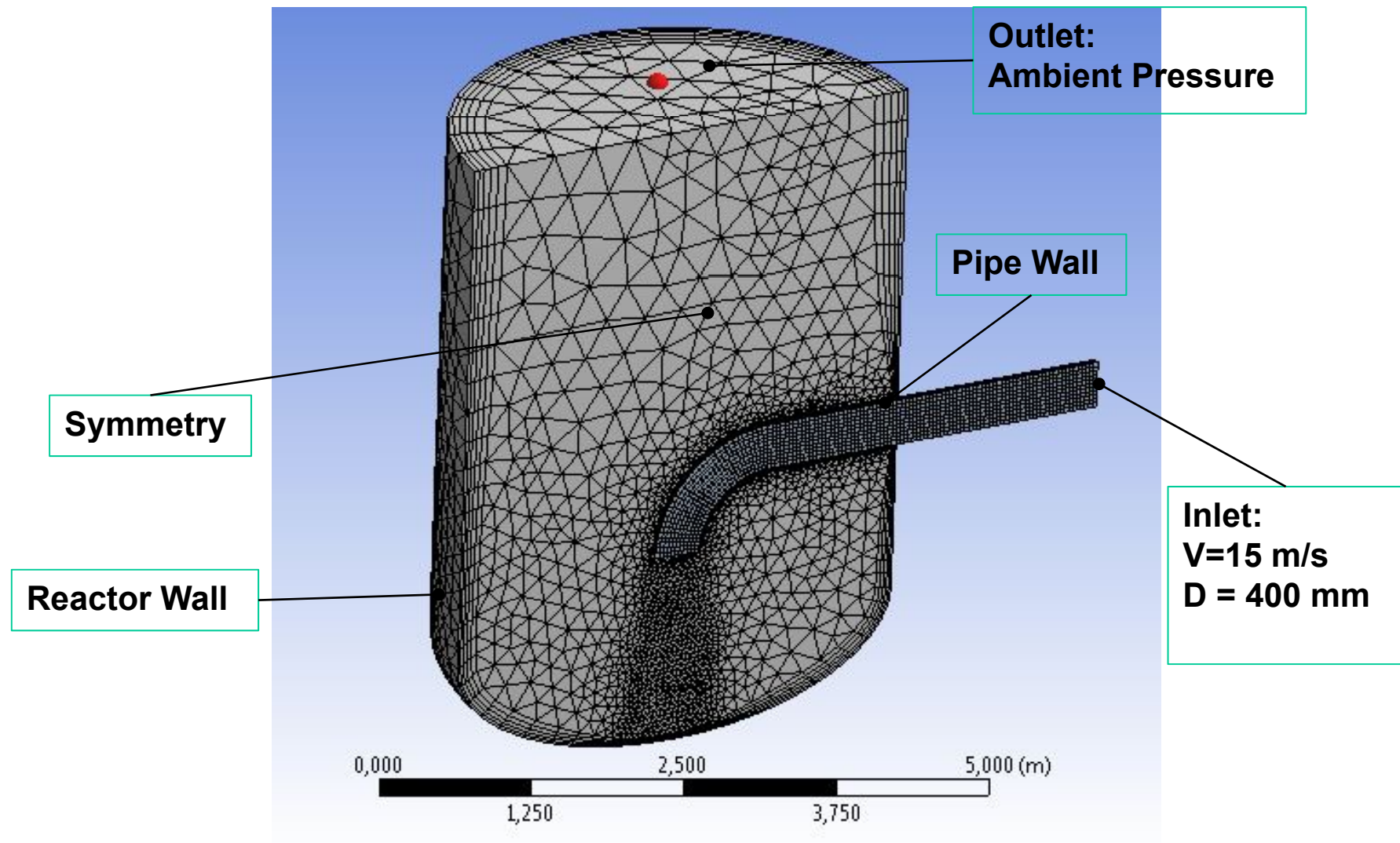
Introduction to ANSYS FLUENT



- **Introduction and Problem description**
- **Mesh**
- **Setup for Single Phase**
 - Models
 - Materials
 - Boundary Conditions
- **Setup for Discrete Phase Model**
 - Models
 - Materials
 - Boundary Conditions
- **Solver Settings**
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Introduction and Problem Description

- Process Gas and Liquid Droplets come into a Reactor
- We will use the Discrete Phase Model (DPM) to track the Liquid Droplets
- For the process, it is important that only small droplets come into the Reaction Zone, to avoid blockage in the catalyst
- If droplets hit the Reactor Wall, they run down – So, it is not necessary to treat them as droplets after hitting the wall
 - Larger droplets will be removed with this logic and only smaller droplets will stay in the domain and pass through to the outlet which is the inlet to the reaction zone.
- The problem is treated as isothermal.



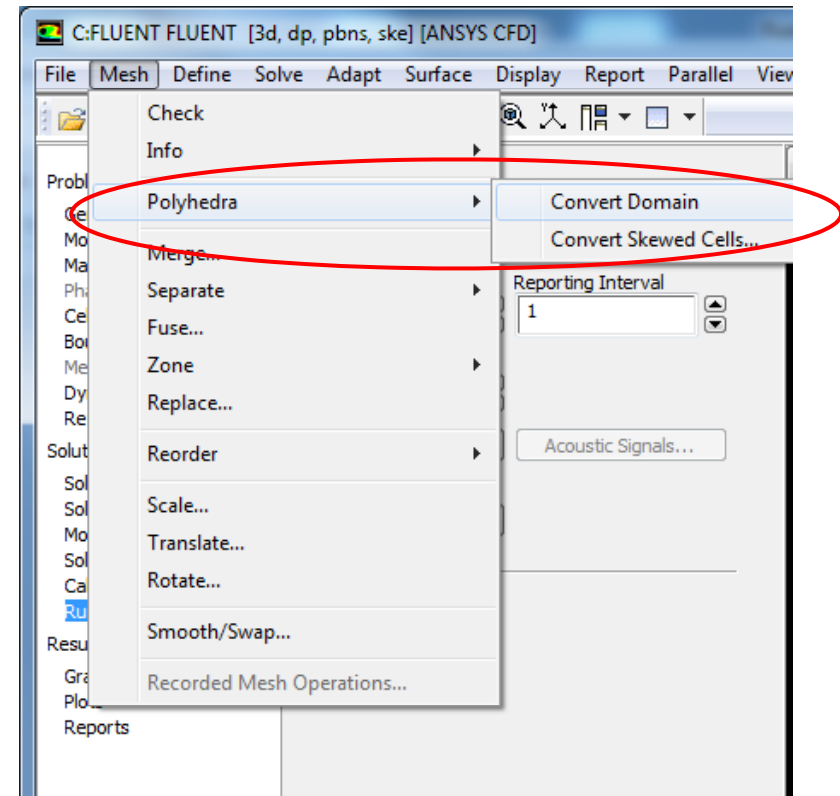
- Launch **FLUENT** running **Double Precision**

We will convert the Tetrahedral elements to Polyhedral elements to reduce the total cell count (so the simulation will proceed more quickly). Since polyhedral cells are less diffusive than the original tetrahedral cells, this should not reduce the overall accuracy.

- Take the option (see Image):
 - **Mesh > Polyhedra > Convert Domain**

The cell count is reduced to 45,000 from the previous 101,000

- Re-display the mesh to see the effect



Setup Single Phase (1)

- **General-**

- Enable gravity: -9.81 m/s^2 in **y** direction to include the effect of gravitational force on the droplets

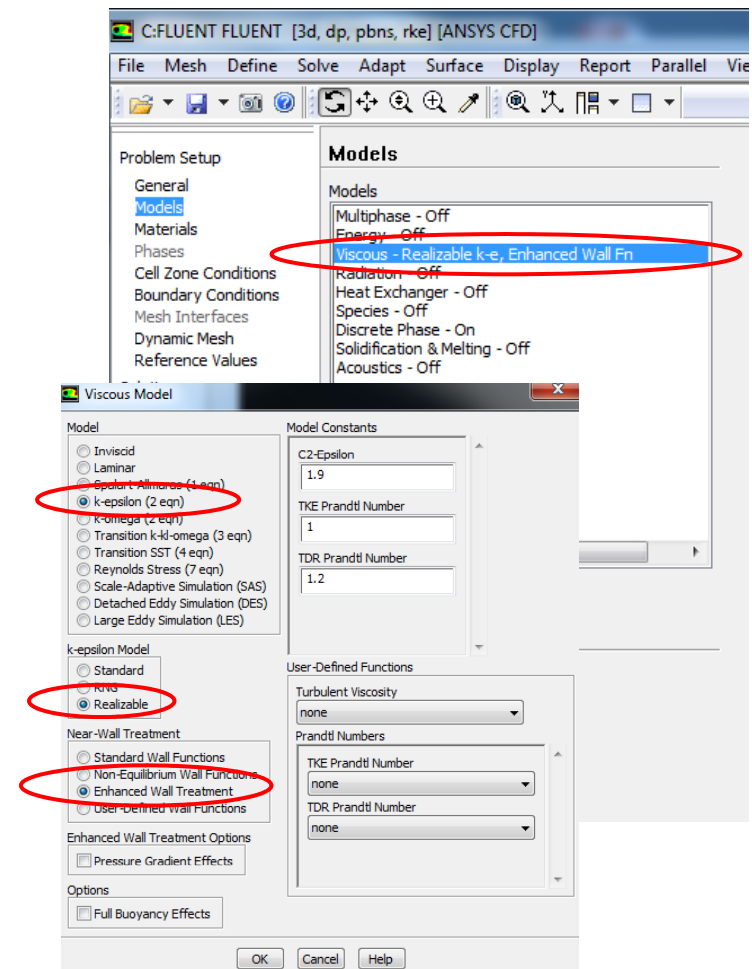
- **Models**

- Turbulent Flow (Re~400,000*)
 - Enable the **Realizable k-epsilon** Model
 - with **Enhanced Wall Treatment**

- **Materials**

- Process Gas assumed to be **Air**

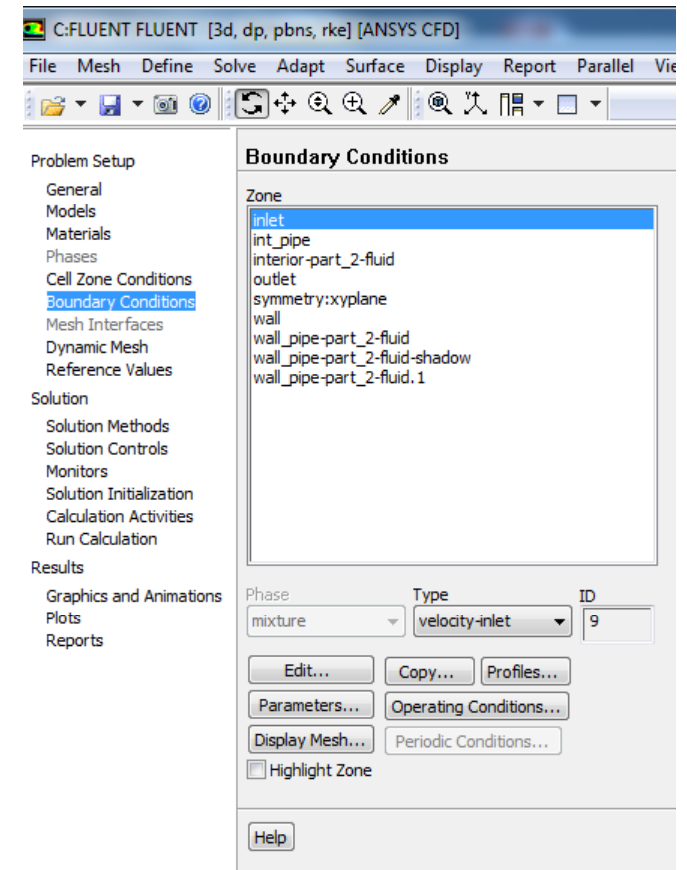
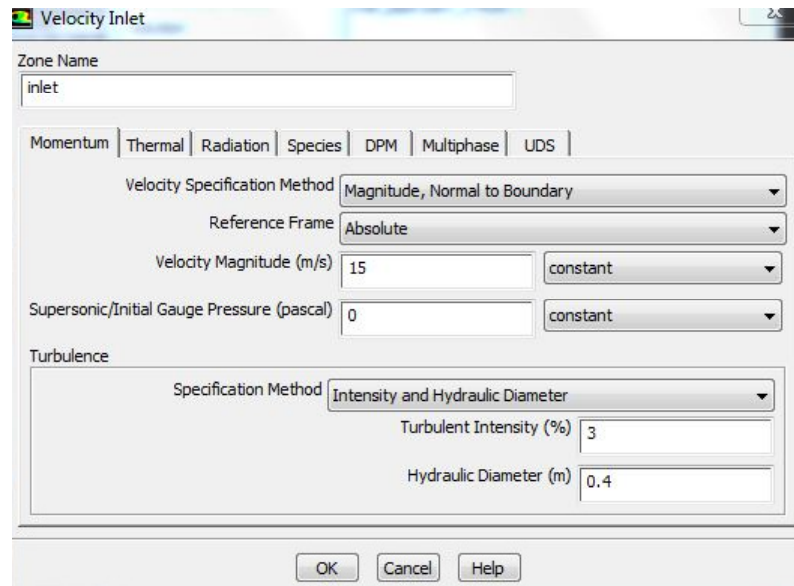
*Assuming process gas as air @STP, $Re = 1.225 \cdot 15 \cdot 0.4 / 1.7894E-5 = 410,752$



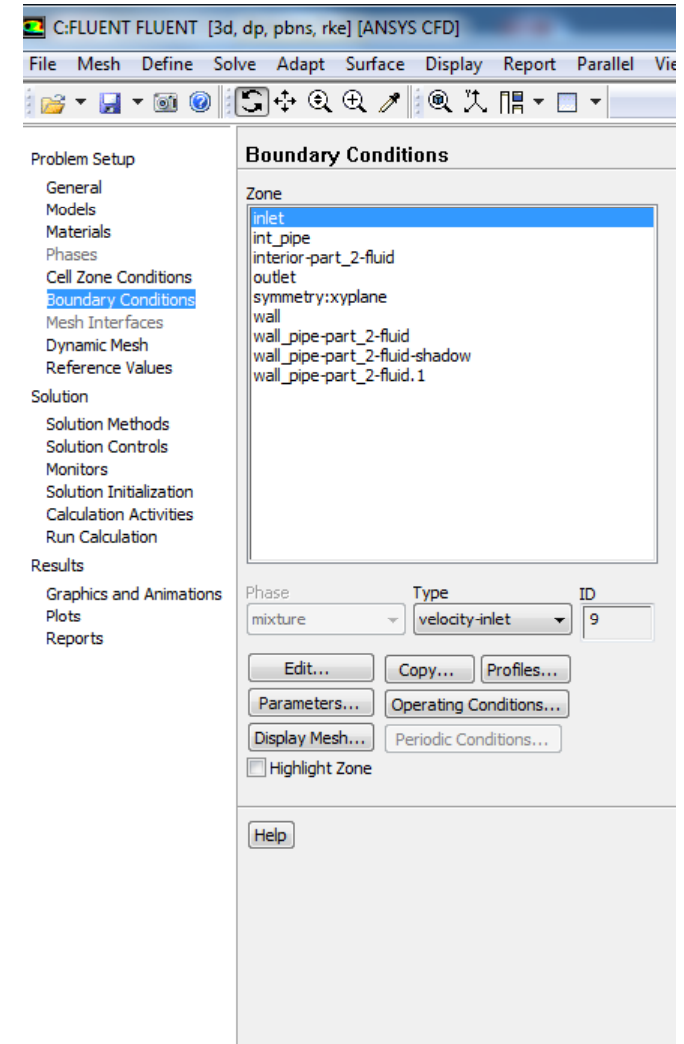
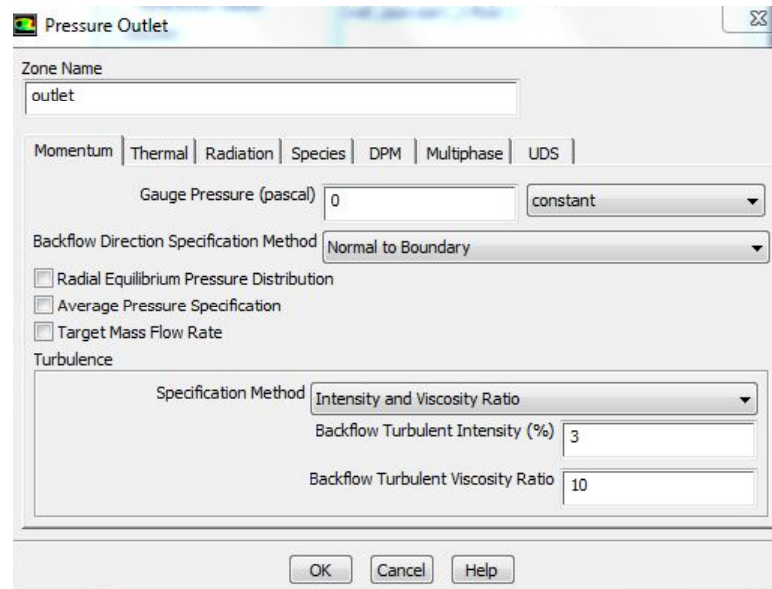
- **Boundary Conditions**

- Define the “Inlet” boundary:

- Type: Velocity Inlet
- Velocity: 15 m/s
- Turbulent Intensity: 3 %
- Hydraulic Diameter: 0.4



- **Boundary Conditions**
 - Define the “**Outlet**” Boundary:
 - Type: Pressure Outlet
 - Gauge Pressure: 0 Pa
 - Backflow Turbulent Intensity: 3 %
 - Backflow Turbulent Viscosity Ratio: 10



Setup Discrete Phase Model (1)



*The **Discrete Phase Model** tracks the motion of individual (discrete) particles. Note that the same principles apply whether the object is a solid particle, or as in this case, a liquid droplet.*

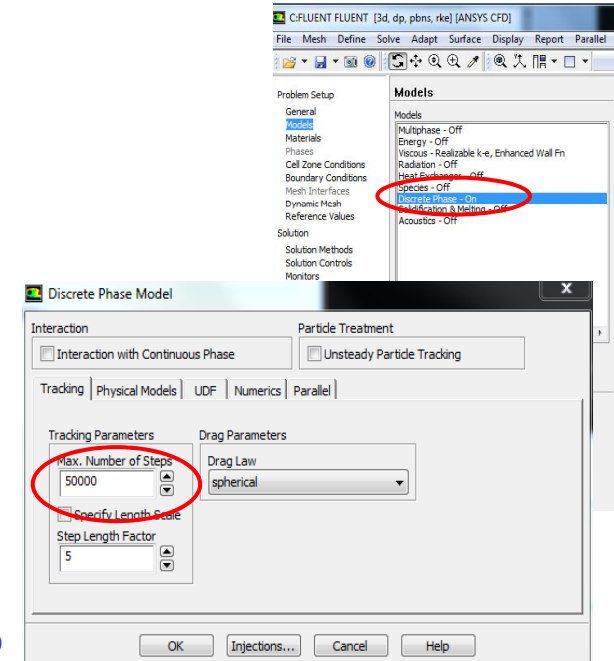
The trajectory of each particle (droplet) is computed over a large number of steps as it passes through the flow domain. Since we know the mass and the surface area of each particle, at each step the solver can compute the balance of forces acting on it. Integrated over the flow domain, the overall trajectory can be determined.

Unlike the continuous phase (air) where material flows through the grid cells (known as an 'Eulerian' reference frame), the DPM moves particles where each particle has its own x,y,z co-ordinate (known as a 'Lagrangian' reference frame).

In this case the particles (droplets) are inert, however the DPM does support much more complex cases where the particles may evaporate and/or combust.

Setup Discrete Phase Model (2)

- **Models > Discrete Phase > Edit**
 - Increase **Max. Number of Steps** to 50000
 - Keep **Step Length Factor** at 5.



The options seen here are:

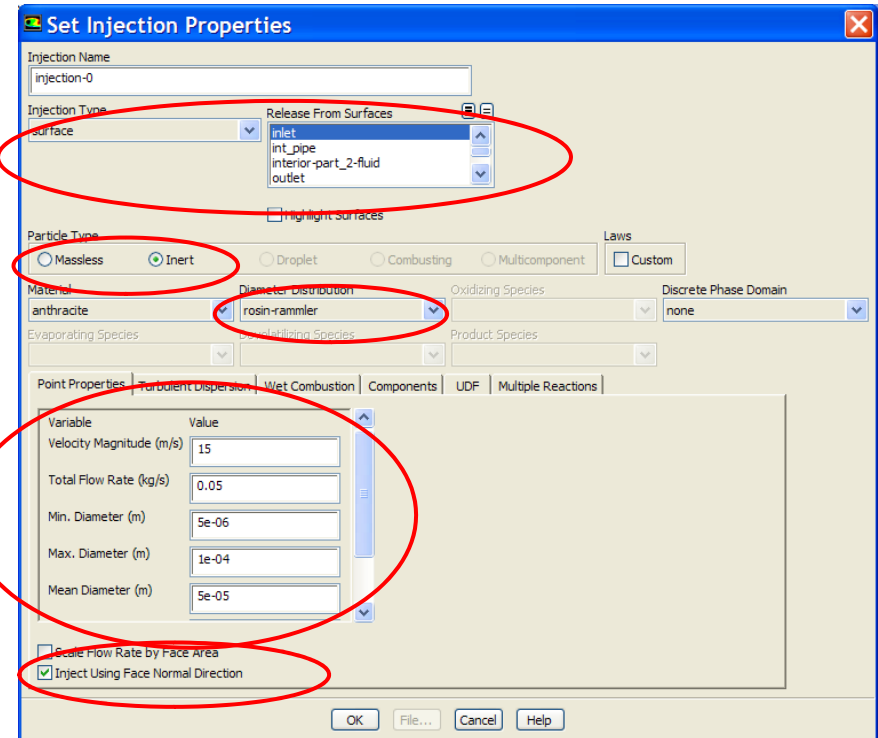
- “*Interaction with Continuous Phase*” – if this was selected (but do **not** select it now) this would mean that as well as the continuous (air) region influencing the particles, the particles will also influence the momentum / energy of the air.
- “*Step Length Factor*” indicates how many steps each particle should make across a grid cell
- “*Max Number of Steps*” sets a limit for the number of steps. Sometimes particles are trapped in a recirculation region, and this parameter is needed to stop the solver being trapped in a continuous loop. Note that if this value is too small, some particles will be terminated too early, before reaching the exit/walls (which will be reported as a high number that are ‘incomplete’)

Setup Discrete Phase Model (3)

• Define – Injections – Create

- Injection Type: Surface
- Release from Surfaces: Inlet
- Particle Type: Inert
- Diameter Distribution: Rosin- Rammler
- Select ‘Inject Using Face Normal Direction’
- Set Point Properties as per table below then ‘OK’ :

Property	
Velocity (normal to inlet)	15 m/s
Mass Flow	0.05 kg/s
Min. Diameter	5e-6 m
Max Diameter	1e-4 m
Mean Diameter	5e-5 m
Spread Factor	3.5
Number of Diameters	20

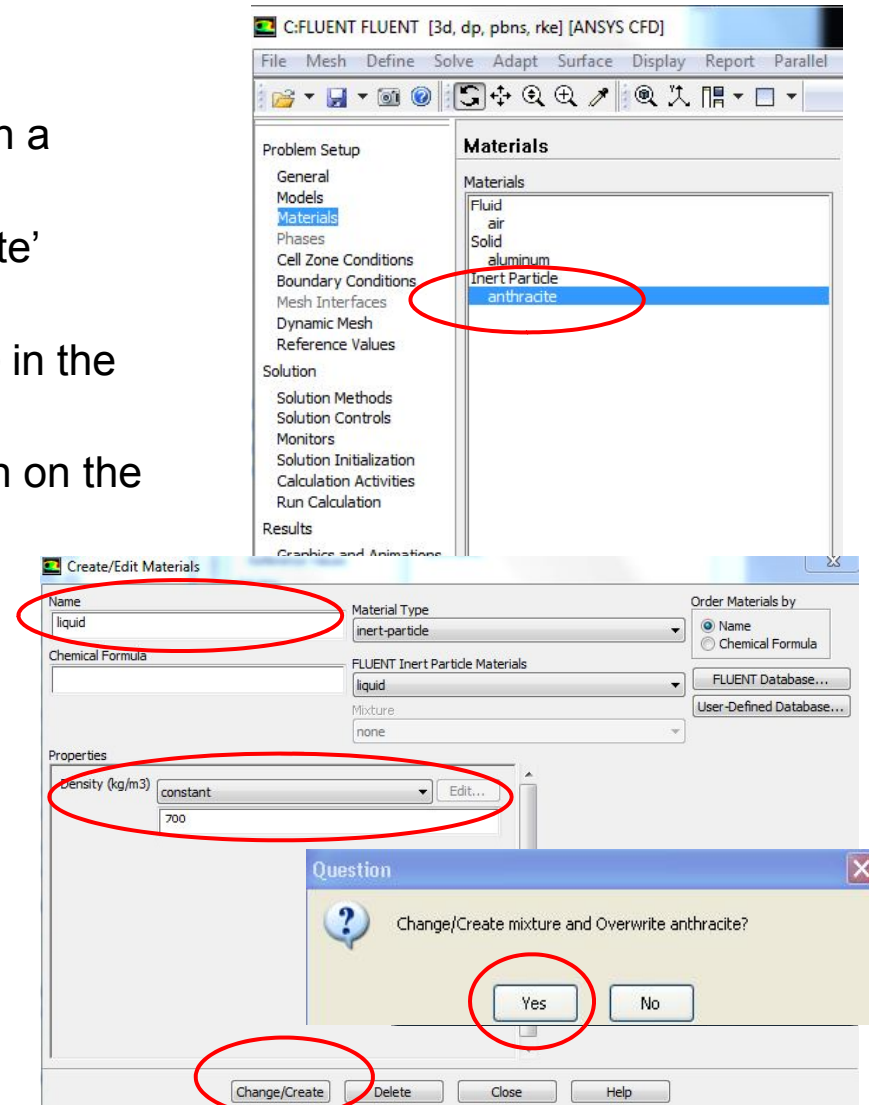


This injection defines the release conditions for the DPM particles/droplets. Note that with a ‘surface’ injection, one particle stream is released from each cell on the ‘inlet’ face. So if (for example) there are actually 10^5 particles, yet only 10^2 cells on the inlet face, then there will only be 10^2 ‘particle streams’ tracked. Each will carry the mass flow rate of 10^3 actual particles (though their trajectories will be based on the mass / diameter of a single particle)

Setup Discrete Phase Model (4)

- **Materials**

- We want to simulate liquid droplets with a density of 700 kg/m^3
- Currently we have the default 'anthracite' particle material.
- To adjust this, *Double Click **anthracite*** in the Materials panel
- Setup new Name and Values as shown on the image
- Store information by *clicking **Change/Create***
- Click Yes to overwrite anthracite.



Setup Discrete Phase Model (5)

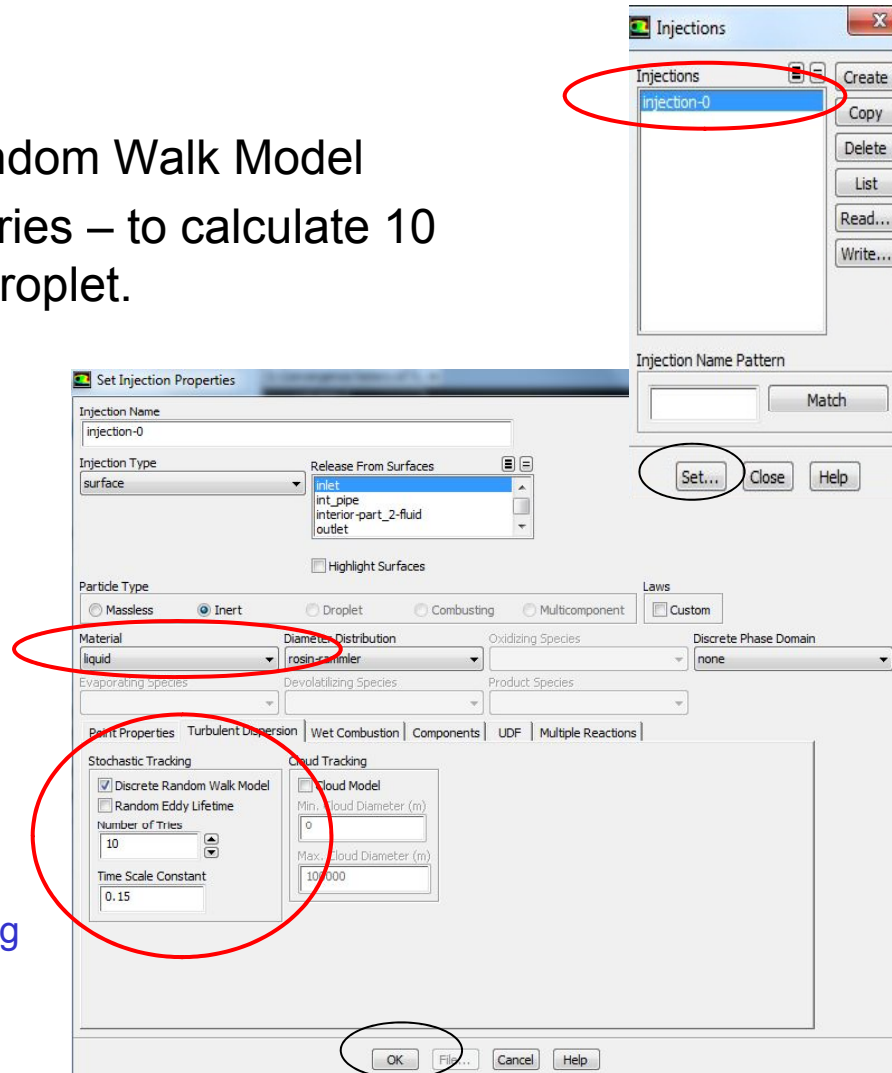
• Turbulent Dispersion

- Activate the Discrete Random Walk Model
- Enter 10 for Number of Tries – to calculate 10 possible paths for each droplet.

To account for the random-ness of the turbulent motion, each particle can be given a 'kick' based on the local turbulent intensity.

"10 Tries" means that 10 releases will be made from each point to see the scatter imparted by the turbulence.

Referring to the example in the commentary on an earlier slide, there would now be 10^3 ($10^2 \times 10$) particle streams tracked, with each now carrying the mass of 10^2 particles (10^5 actual droplets divide by 10^3 particle streams)



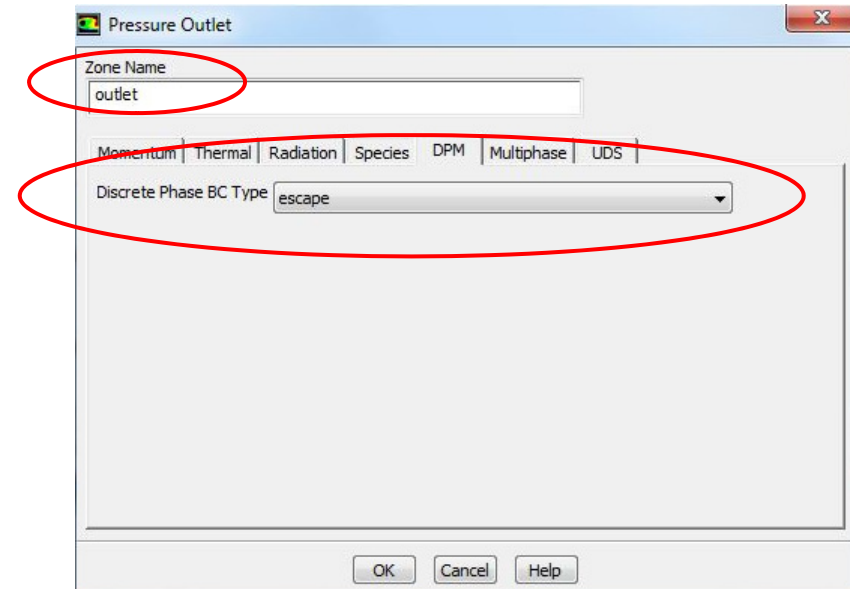
Setup Discrete Phase Model (6)

The solver needs to know what to do with a DPM particle / droplet when it meets a flow boundary. Note the additional 'DPM' tab on the Boundary condition panels for this. The main choices are:

- 'Escape' if particles are free to leave at this boundary
- 'Reflect' if they will bounce off this boundary
- 'Trap' if they will stick to this boundary

• DPM Boundary Conditions:

- Set the DPM conditions for the boundaries as per the table below:



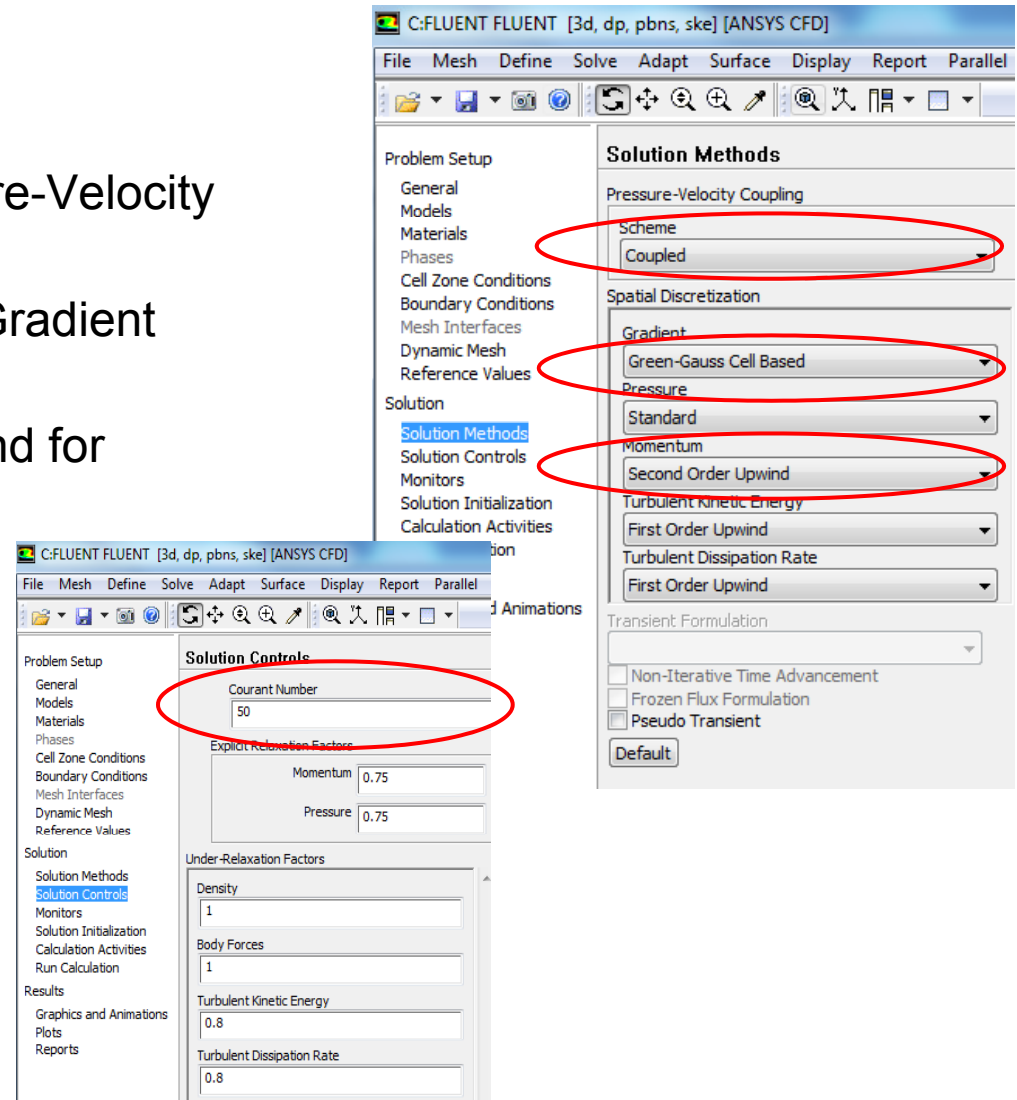
Boundary	DPM BC	Physical Meaning
inlet	escape	-
outlet	escape	Particle leaves the domain – Tracking ends
wall	trap	Particle is removed but its current mass and energy is imparted to the gas phase.
wall_pipe-[*]	reflect	Particle rebounds off of the pipe wall with the normal and tangential coefficients of restitution set in the reflect panel.

- **Solution Methods**

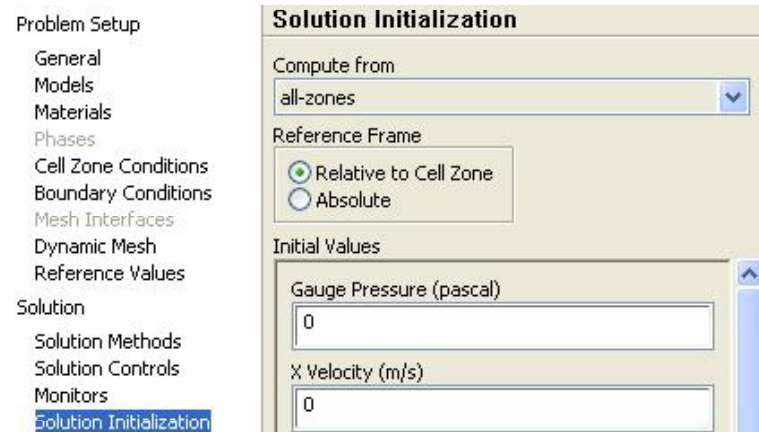
- Switch to **Coupled** for Pressure-Velocity Coupling
- Green-Gauss Cell Based for Gradient Discretization
- Switch to Second Order Upwind for Momentum

- **Solution Controls**

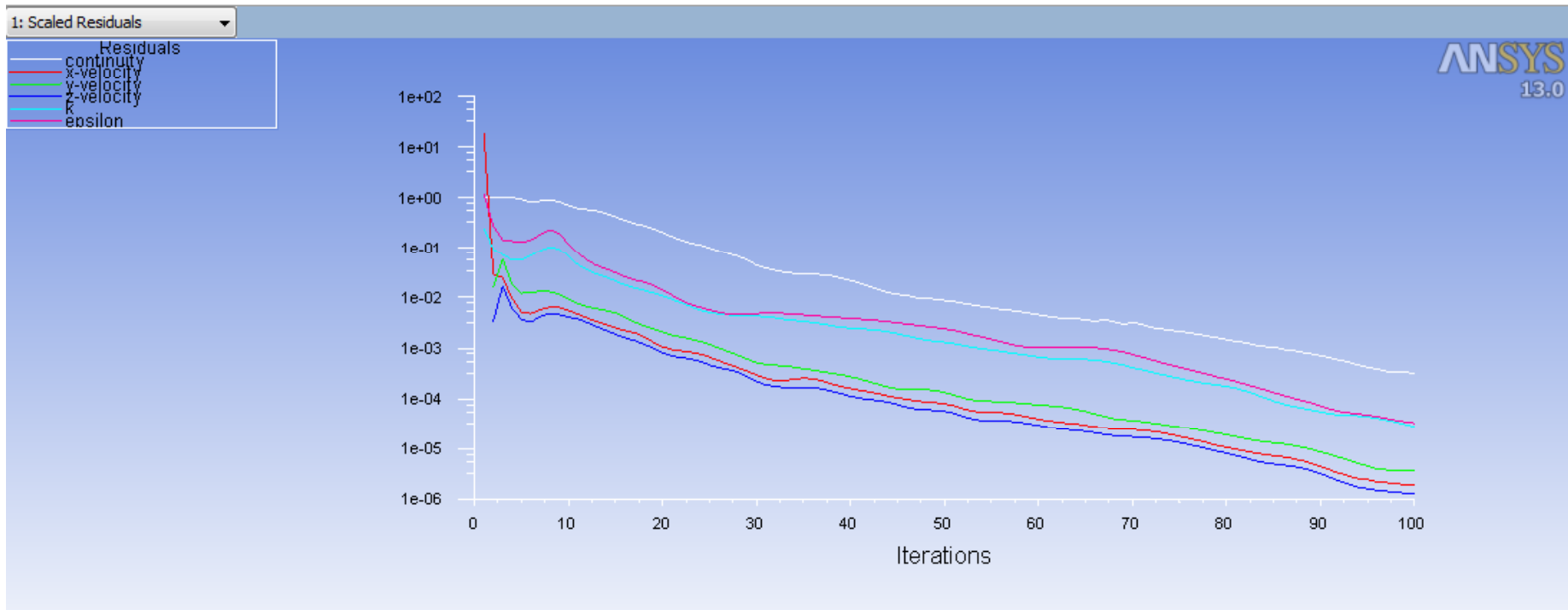
- Decrease the Courant Number to **50**



- **Monitors:**
 - **Residuals** : Set Convergence Criteria to 'none'
- **Initialize – Compute from all-zones**



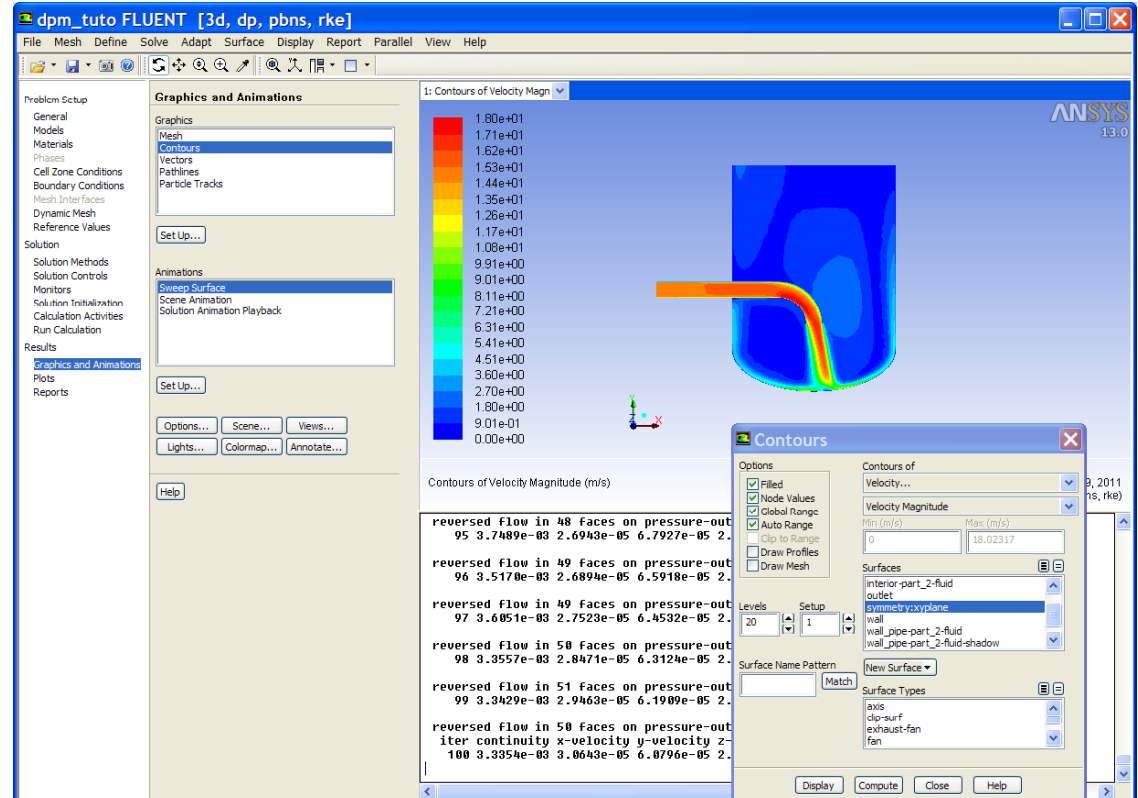
- Run the model for 100 Iterations



Recall that we did not select 'Interact with Continuous Phase' when setting up the DPM. The trajectories have not yet been computed, all we have currently solved for is the movement of the continuous phase (air). The DPM computation will happen when we post-process the particle trajectories.

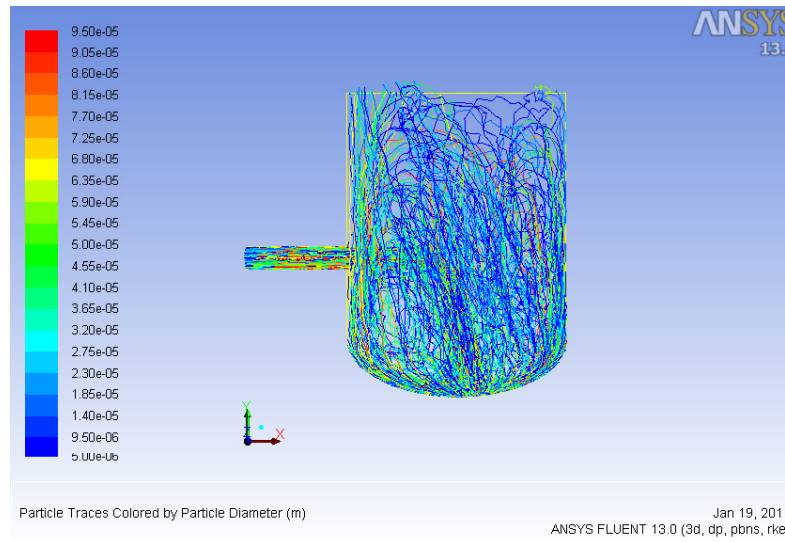
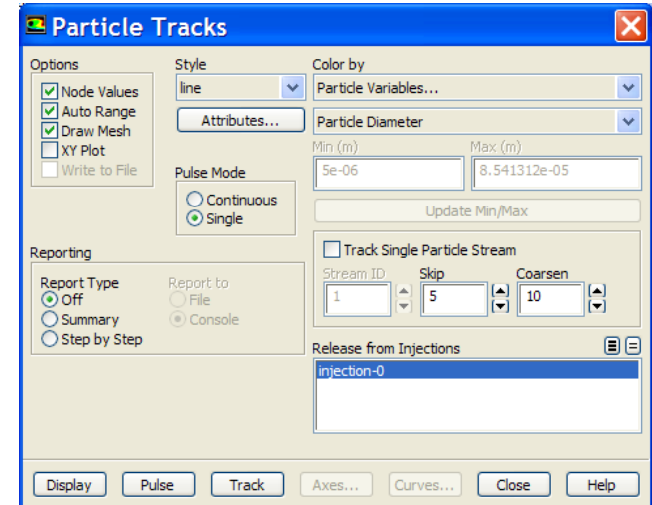
However if we had selected 'Interact with Continuous Phase', then at every pre-defined number of iterations, the DPM particles would have been tracked. These would have provided a revised momentum source/sink for the air, and as a result we would see spikes in the residuals at each DPM computation.

- **Display Velocity Contours:**
 - Display contours of the Velocity Magnitude at the Symmetry plane
- Align view angle by using:
 - > Views > Front > Apply



• Display Particle Tracks

- Graphics and Animations > Particle Tracks
- Choose Draw Mesh > Symmetry Plane > Edge-Type Outline > Display > Close
- Select 'injection-0' to release from
- Colour by Particle Diameter
- Skip Tracks by 5
- Coarsen each track by 10 (only every 10th calculated Point on a track will be displayed)
- Select 'Display' and wait



- At this point (when pressing 'Display' on the previous slide) the DPM iteration is performed. The status of this is shown in the TUI window:

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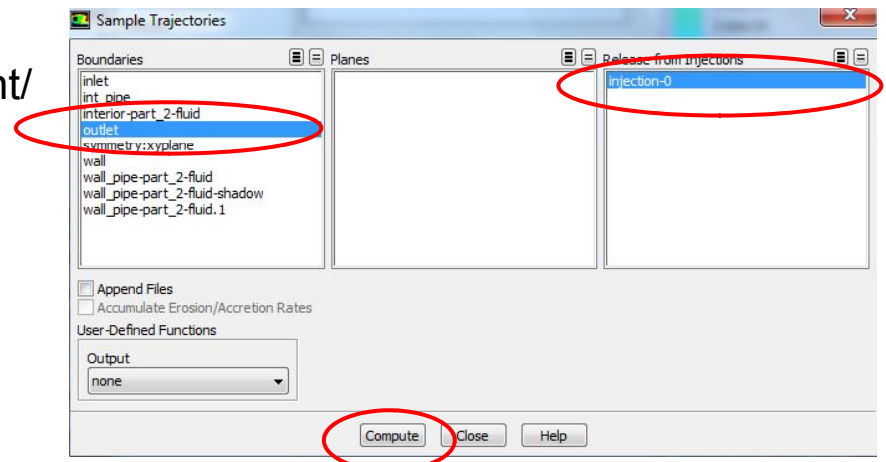
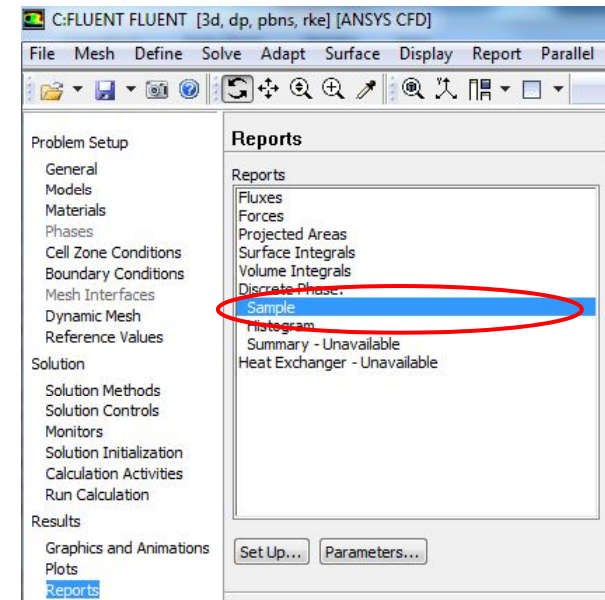
Particle Traces Colored by Particle Diameter (m)
Jan 19, 201
ANSYS FLUENT 13.0 (3d, dp, pbns, rke)

98 3.3557e-03 2.8471e-05 6.3124e-05 2.1896e-05 1.1220e-03 1.6773e-03 0:00:03 2
reversed flow in 51 faces on pressure-outlet 6.
99 3.3429e-03 2.9463e-05 6.1909e-05 2.2872e-05 1.1393e-03 1.7575e-03 0:00:01 1
reversed flow in 50 faces on pressure-outlet 6.
iter continuity x-velocity y-velocity z-velocity k epsilon time/iter
100 3.3354e-03 3.0643e-05 6.0796e-05 2.3996e-05 1.1687e-03 1.8541e-03 0:00:00 0
number tracked = 1870, escaped = 51, aborted = 0, trapped = 1819, evaporated = 0, incomplete = 0

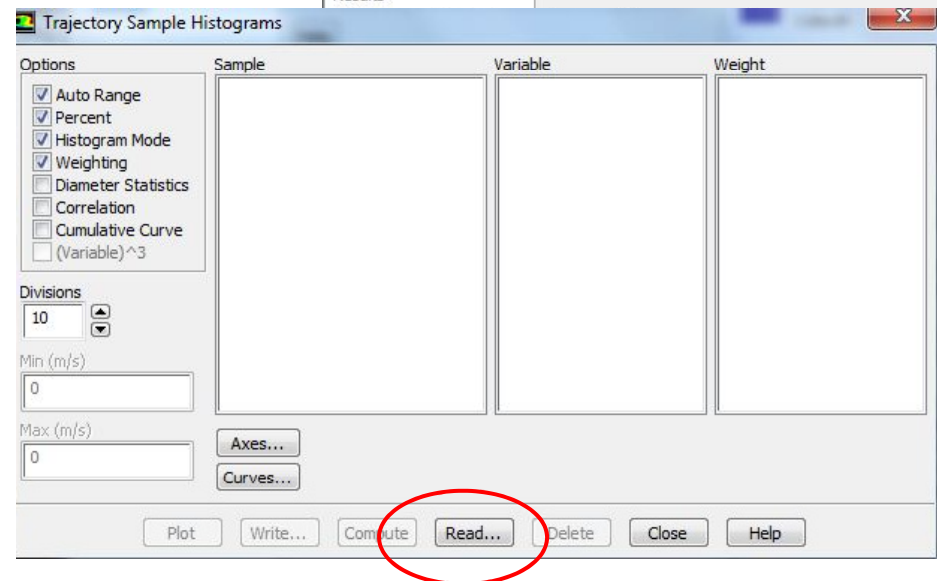
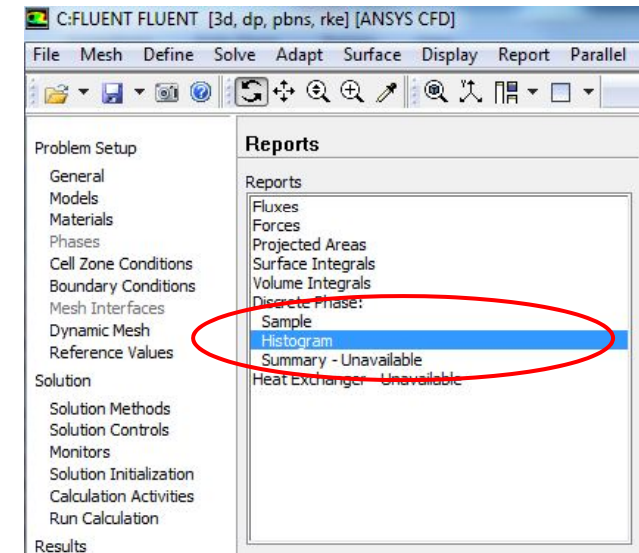
```

- The Number of incomplete particles should be zero. If not, the “Max. Number of Steps” can be increased (Models > Discrete Phase).
- If increasing the steps does not change the number of incomplete particles then particles are quite likely caught in a recirculation zone(s). In this case, revert this setting as it is not efficient to run too many steps for particles that are caught in a recirculation zones.

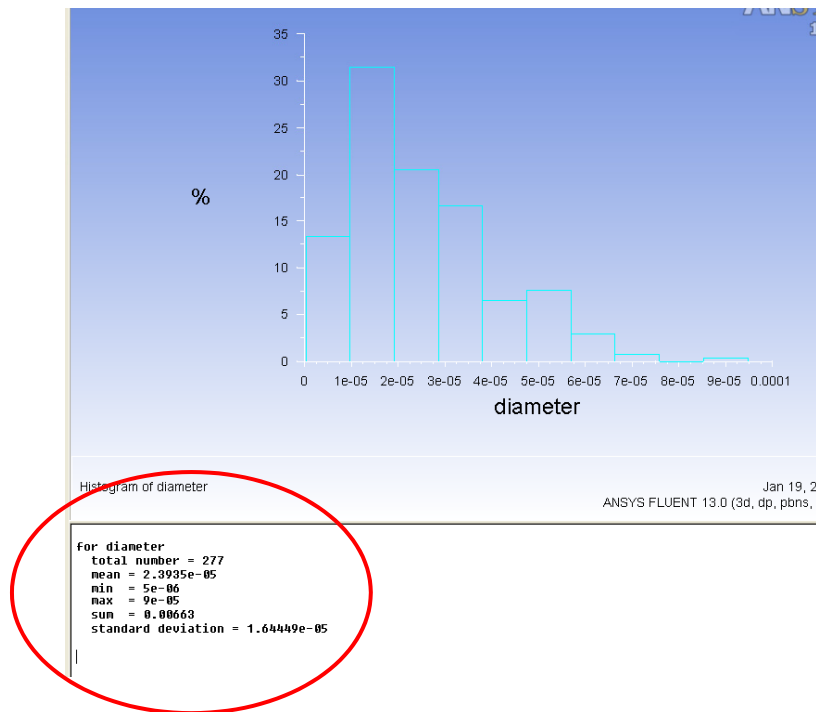
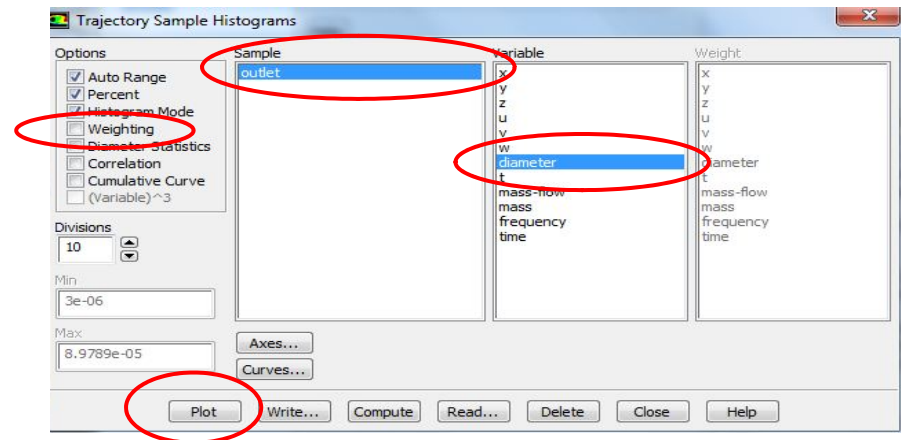
- Obtain the Diameter Distribution at the **Outlet** using the Discrete Phase Sample/Histogram panels
- First, create a DPM Sample File
 - Reports > Discrete Phase > Sample
 - Select 'outlet', 'injection-0' and 'Compute'
 - Whenever a Particle passes a chosen Zone, its current properties will be written out to a file [zone name].dpm
 - The Files are located where FLUENT case and data files are stored (for WB Usage: [WB_project_name]_files/dp0/FLU/Fluent/outlet.dpm)



- Second, display this sample file using the Histogram option.
- Reports > Discrete Phase > Histogram
- Click the Read button.
 - A File browser will open; select the sample file that was just created (outlet.dpm)

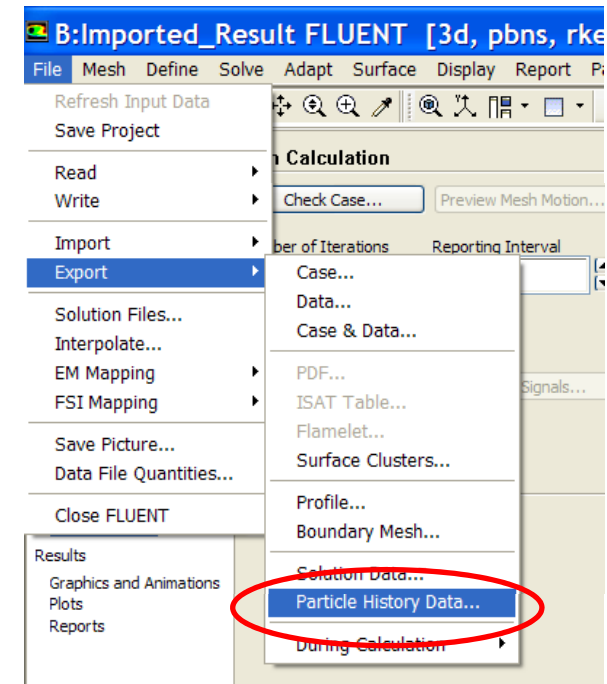
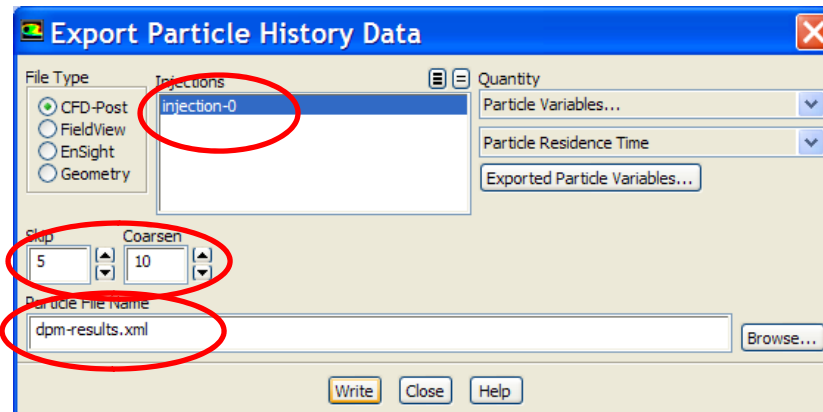


- Switch off the *Weighting* and select *diameter* under the Variable column.
- Click Plot to see a bar chart of the diameter bins at the outlet.
 - In TUI Console, you can see some statistical details



Appendix - Post-processing in CFD-Post

- You can read the case and data files in CFD Post but, in order to visualize the Particle Tracks in CFD Post, you need the Track file
 - File > Export > Particle History Data
 - Select 'injection-0'
 - Set 'Skip' to 5, and 'Coarsen' to 10
 - Particle Filename : 'dpm-results.xml'
 - 'Write'



Recall that the DPM trajectories are computed in their own Lagrangian reference frame – in other words the trajectories are not part of the normal “fluid” data stored for each grid cell. As a result, the DPM trajectories are not saved as part of the FLUENT case & data file. If these are to be post-processed in CFD post, the DPM “Particle History Data” needs to be exported as a separate file.

Appendix – Post-Processing in CFD-Post[2]

- Save your Case & Data (or Project if in Workbench)
- Close FLUENT
- [If in Workbench] Right-click on the solution cell, and select “Transfer Data to New” then “Results”. Double-click on ‘Results’ to launch CFD Post
- [If standalone] Launch CFD-Post, and read in the case and data file.
- [Both Methods, in CFD-Post] File > Import > Import FLUENT Particle Track File.
- Select the file saved on the last slide “dpm-results.xml”.

If in Workbench, this will be :

`[WB_project_name]_files/dp0/FLU/Fluent/dpm-results.xml`

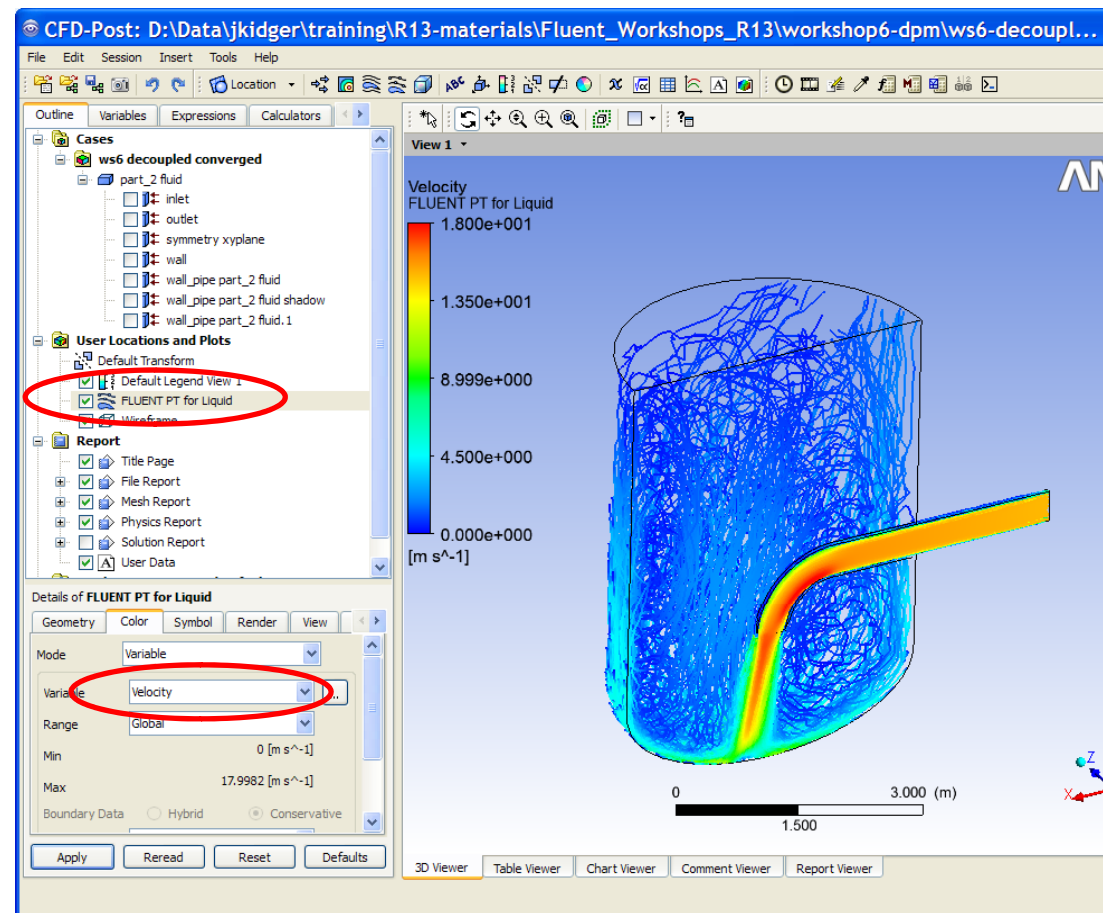
- A new item appears in the model tree “FLUENT PT for Liquid”
- To re-create the image shown, increase the “Maximum Number of Tracks” to 2000, and colour by Velocity then ‘Apply’

In this case there were 1120 mesh faces across the inlet. We used turbulent tracking with 10 tries.

Hence if FLUENT simulated all trajectories, that would be 11200 particle tracks computed.

When we exported the dpm data from FLUENT, we applied a ‘skip’ of 5 (so only every 6th line is exported). Hence the data file will contain 1870 trajectories.

By setting max tracks to 2000 we plot everything in the data file. If you increase this value, no additional tracks are displayed.



In this example, we chose to only offer one-way coupling between the fluid (air) and the droplets. The air flow influenced the particles, but not the opposite. The particle motion had no influence on the air flow. By doing this the workshop could be run fairly quickly.

However you may be concerned that the loading of the droplets may be significant, and their presence may modify the air flow pattern. To check this, try computing with coupled motion

In the FLUENT setup:

- Go to Models > Discrete Phase
- Set 'Interact with Continuous Phase'
- Set 'Number of Continuous Phase Iterations' to 20, then 'OK'.
- Run the simulation for a further 250 iterations (or for however much time you have) and repeat the post-processing

