

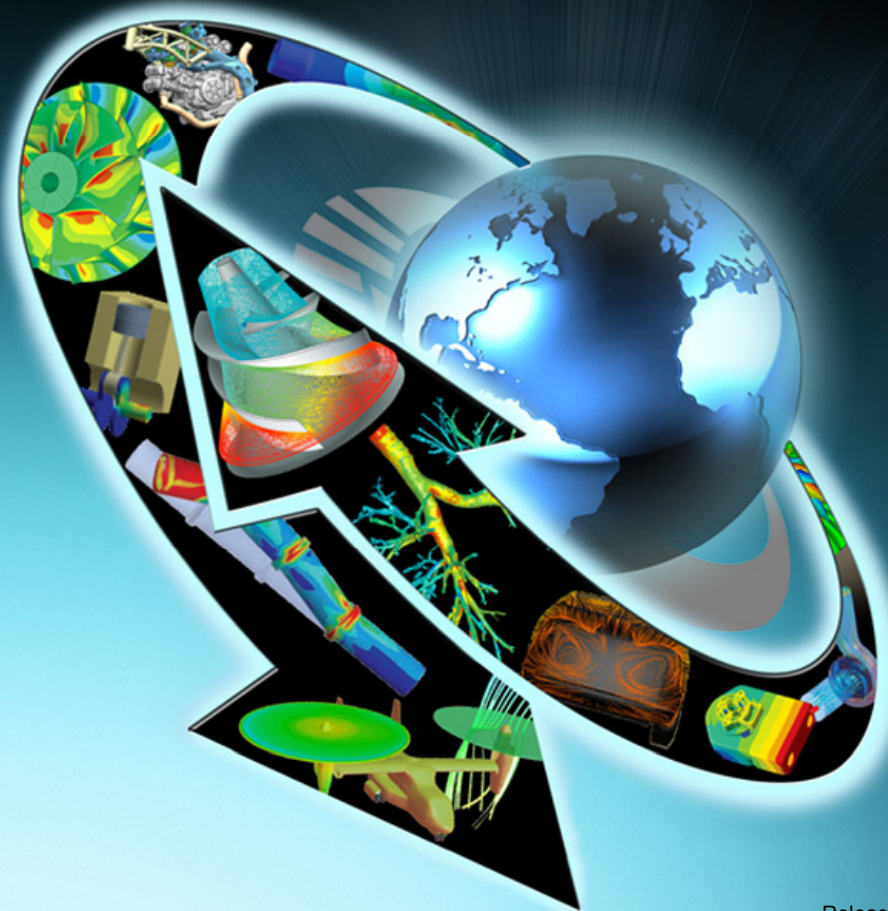


Customer Training Material

Workshop 3

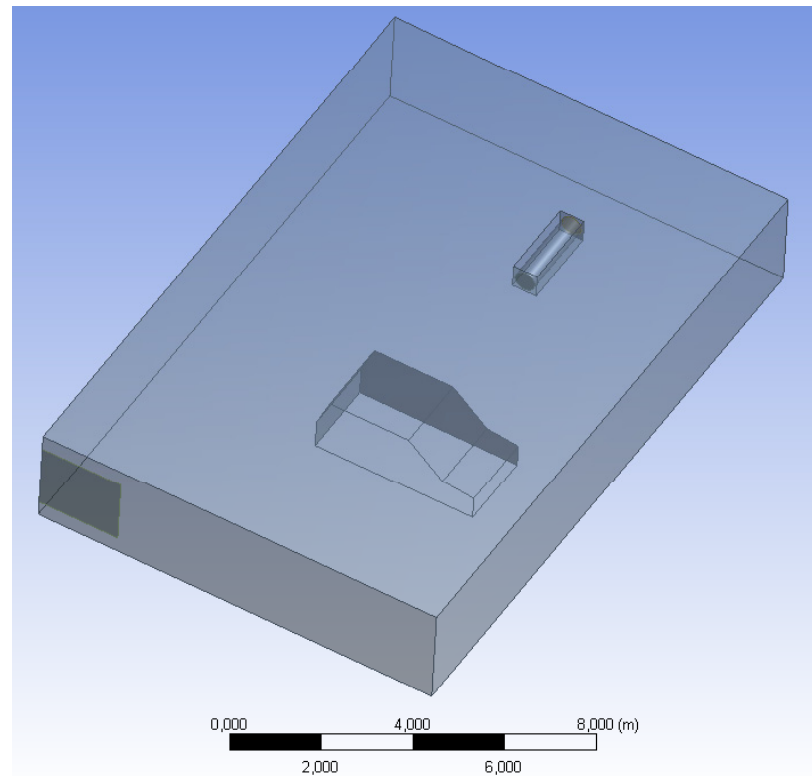
Modeling Multi-Species Flow

Introduction to ANSYS FLUENT



Introduction (1)

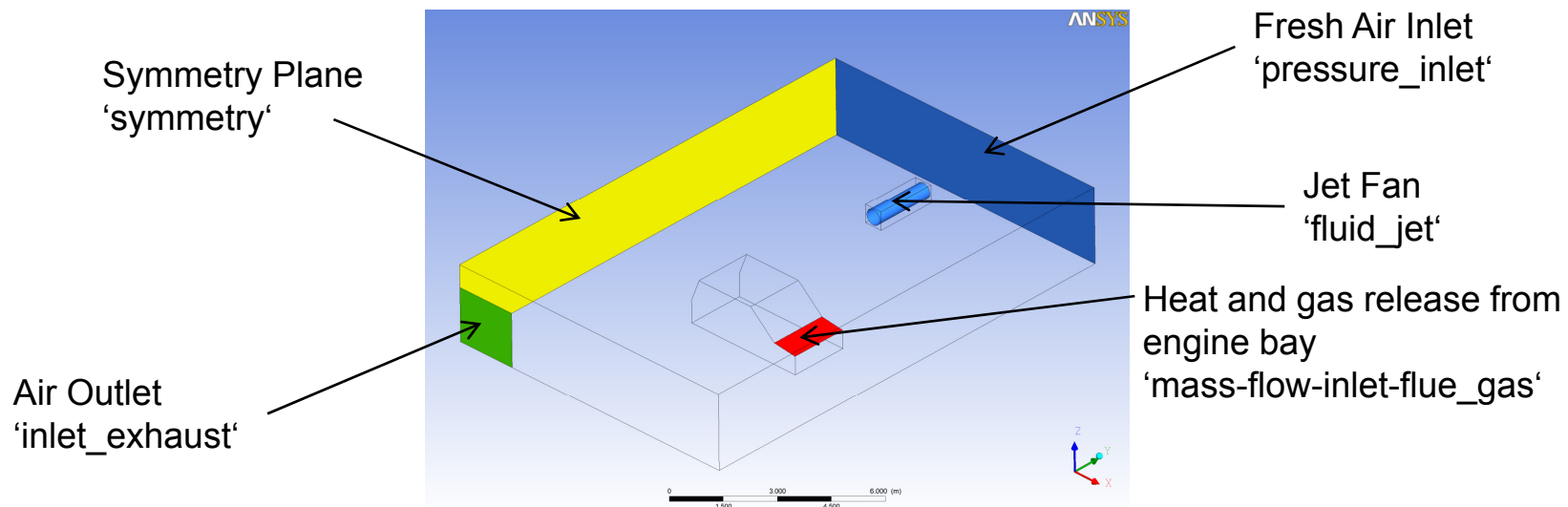
In this workshop you will analyze the release of heat and combustion gases from a single car with an engine fire in a ventilated parking garage. The simulation will be run as a steady state analysis assuming the fire has reached a stable developed stage.



Introduction (2)

- Simulation Physics & Boundary Conditions

- Mixture of N_2 , O_2 , CO_2 and H_2O
- 6 m/s exhaust
- 80 N/m^3 momentum source in jets
- 0.1 kg/s flue gases (H_2O and CO_2) at 1200 K
- k-epsilon turbulence model
- DO radiation model with WSGGM for absorption coefficient
- 300 K inlet temperature



Goals

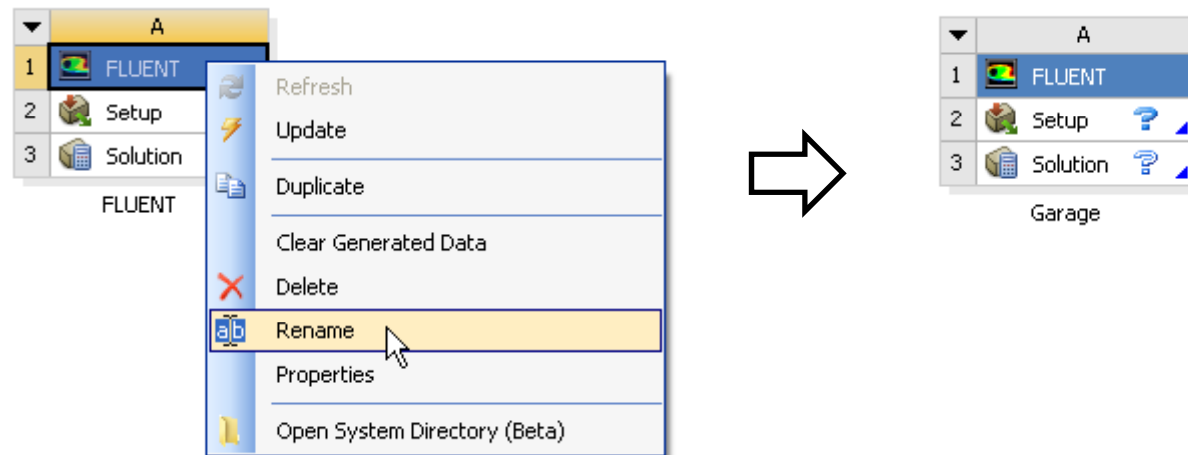
- This Workshop will demonstrate how to:
 - Set up a case with multiple species
 - Define absorption coefficient for flue gases
 - Define gravity and operating conditions for buoyancy driven flows
 - Define volumetric sources
 - Change solver settings and boundary conditions during the calculation by using calculation activities
 - Judge solution convergence using monitors
 - Postprocess a case with multiple species

- Files

- Copy the following files to your working directory.
 - garage.msh
 - calc_activities.jou
 - multi-species-solved.wbpz

Starting Workbench

- Open Workbench
 - Start > Programs > ANSYS 13.0 > ANSYS Workbench
 - Drag a FLUENT Component System into the project schematic
 - Rename the system to 'Garage' (RMB on cell A1 to rename the system)



- Manage External Files

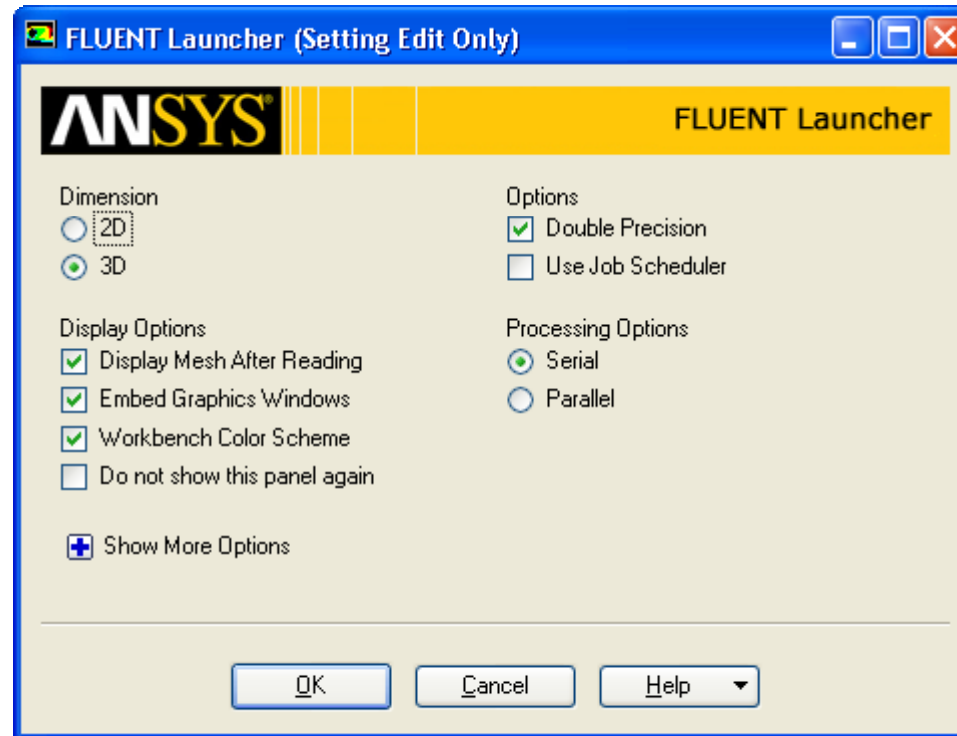
- This project requires the import of existing files. Workbench creates a directory named 'User Files' where files created externally can be stored and associated with the project.
 - This enables Workbench to synchronise projects with external files.
- From the Workbench project page save the project to your working directory using the name "multi-species".
 - The 'user_files' directory will be found in the project files directory.



- Copy the two files "garage.msh" and "calc_activities.jou" to this directory. All files associated with the project are listed when the Files option is checked from the Workbench View menu.



- Start FLUENT
 - Double click on the Setup cell to open FLUENT
 - Choose 3D and Double Precision under Options and retain the other default settings (if your computer has 2 or more nodes and parallel licenses are available, you also could start FLUENT parallel)

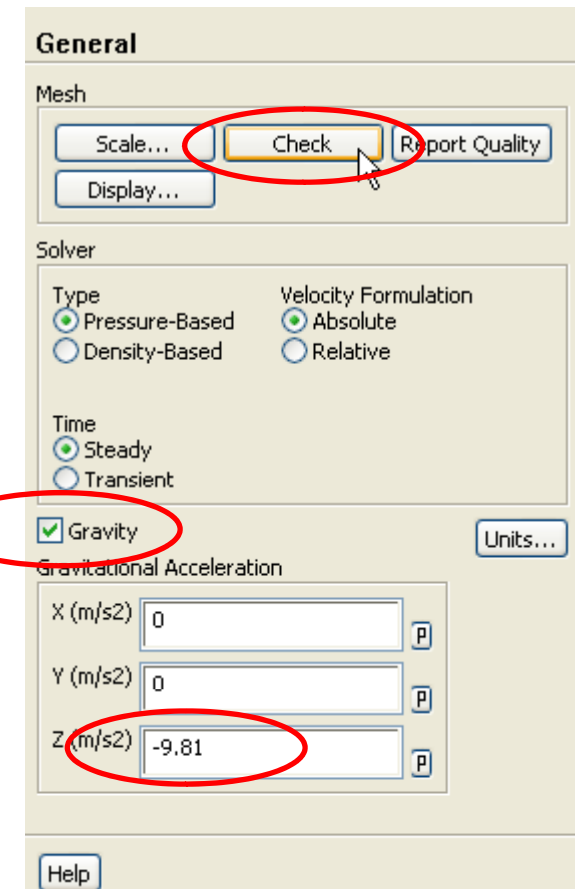


Import Mesh and General setup

- Import the existing mesh file
 - Under the Fluent File menu select Import > Mesh.
 - Select the file 'garage.msh' and click OK to import the mesh.
 - To check for any problems in the mesh click Check. There should be no problems reported in the TUI window.

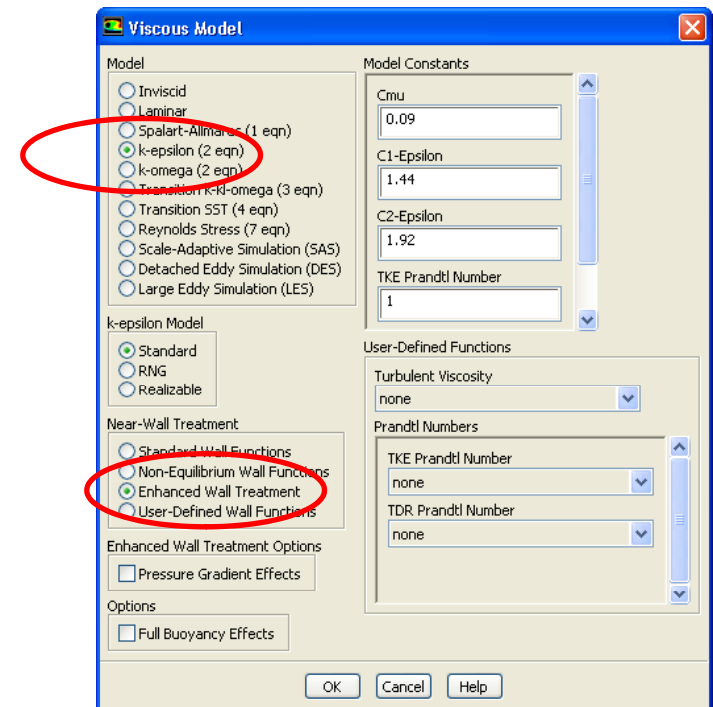
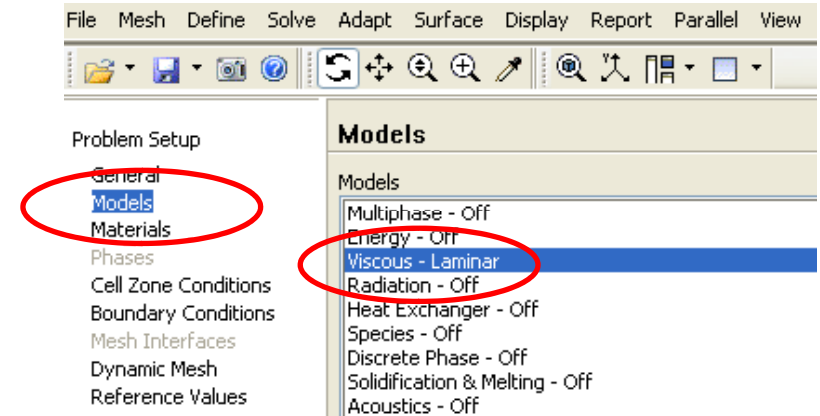
Checking mesh.....
Done.

- Reorder the mesh using Mesh > Reorder > Domain (from the menu).
 - Reordering the domain can improve the computational performance of the solver by rearranging the nodes, faces and cells in memory.
- Retain defaults for the solver
- Enable gravity and set $z = -9.81 \text{ m/s}^2$



Setting Physics (Turbulence)

- Specify turbulence model
 - Select Models in the navigation pane.
 - Double click Viscous in the model selection pane. The Viscous Model panel will open.
 - Select k-epsilon (2 eqn) under Model, Standard under k-epsilon Model and Enhanced Wall Treatment under Near-Wall Treatment.
 - Turbulence modelling, as with all physics modelling, is a complex area. There are many application specific options. The documentation provides further guidance on which models to use for specific applications.
 - Click OK



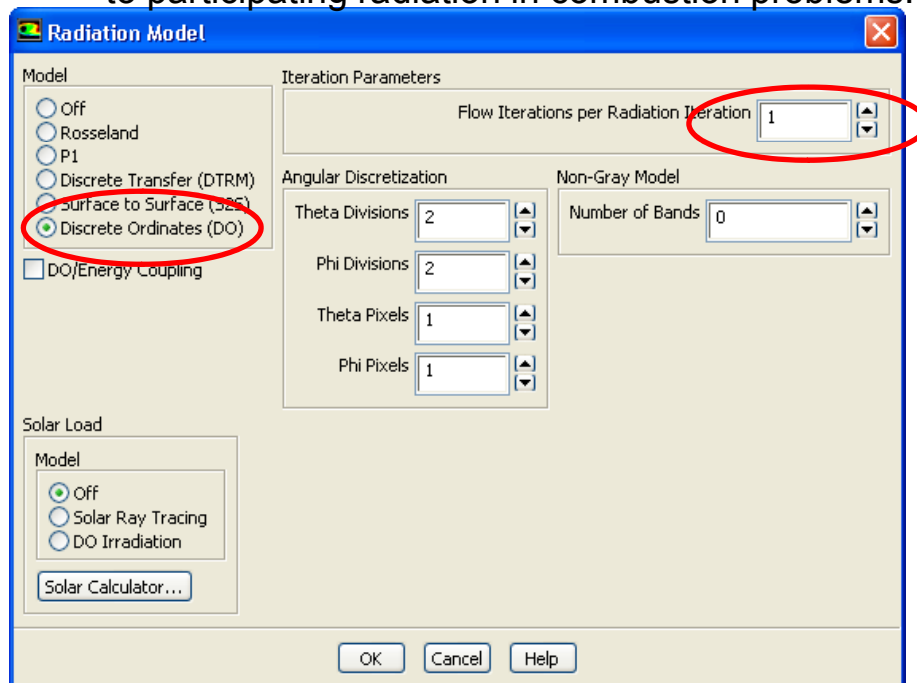
WS3: Modelling Multi Species Flow

Setting Physics (Radiation)

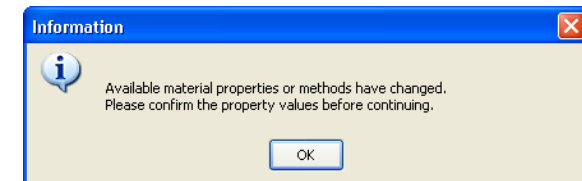


- Specify radiation model

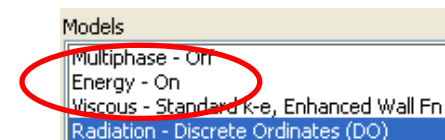
- Double click Radiation in the model selection pane. The Radiation Model panel will open.
- Select Discrete Ordinates (DO) under Model.
- Set Flow Iterations per Radiation Iteration to 1 and click OK.
 - ANSYS FLUENT provides five radiation models. The DO model spans the entire range of optical thicknesses, and allows you to solve problems ranging from surface-to-surface radiation to participating radiation in combustion problems.



You will be informed, that material properties or methods have changed. The Text User Interface (TUI) will list new material properties required for radiation modelling. Click OK. Material properties will be defined later.



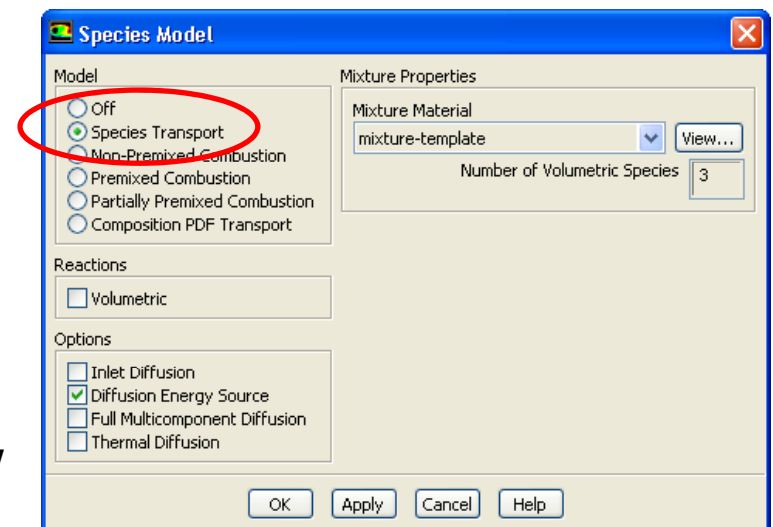
Note also that the energy equation is switched on automatically when any heat transfer related physics are requested.



Warning: Enabling energy equation as required by radiation model.

Setting Physics (Species / Mixture)

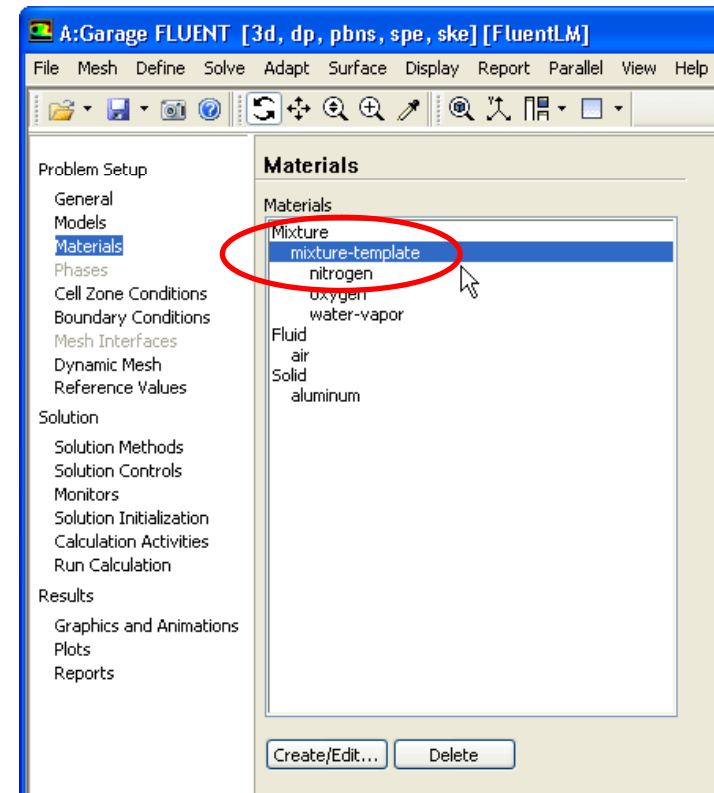
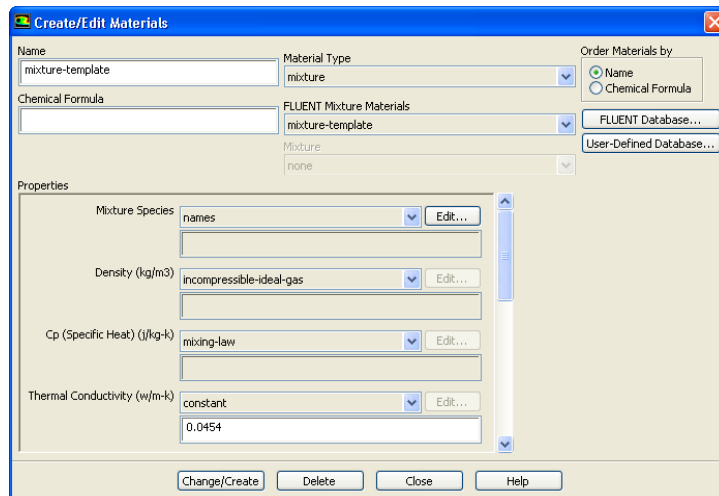
- Specify species model
 - Double click Species in the model selection pane. The Species Model panel will open.
 - In this workshop the products of combustion (heat & gases) will be modelled rather than the reaction itself.
 - Select Species Transport and click OK.
 - Switching on the species model will, as with the radiation model, introduce new material properties. An information box will appear. Click OK to accept this.
 - This setup will enable the tracking of non-reacting chemical species.



The species model requires the definition of a 'mixture' representing the chemical species of interest. The default mixture contains nitrogen, oxygen and water vapour.

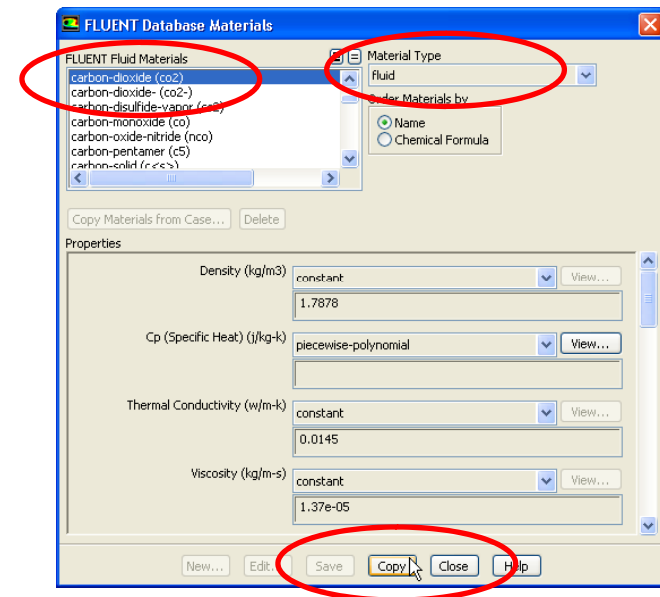
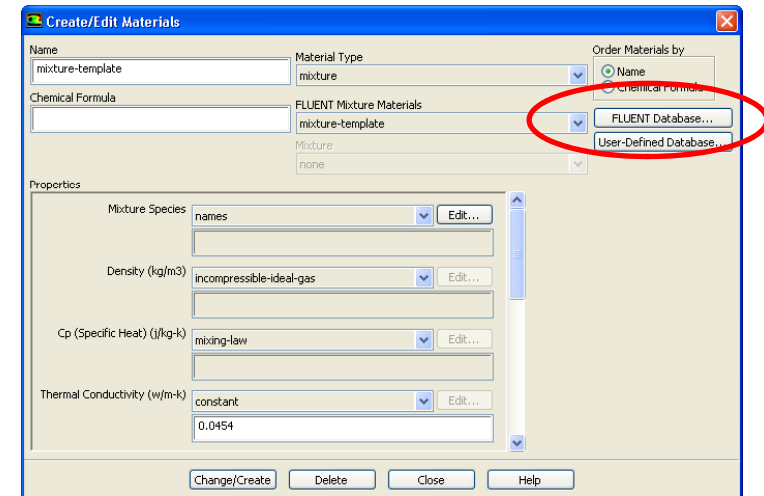
Defining Materials (1)

- Specify mixture
 - Select Materials in the navigation pane.
 - Note that under Mixture in the Materials pane the default mixture is listed as containing nitrogen, oxygen and water-vapour.
 - Double click mixture-template, this will open the Create/Edit Materials panel with the mixture preselected.



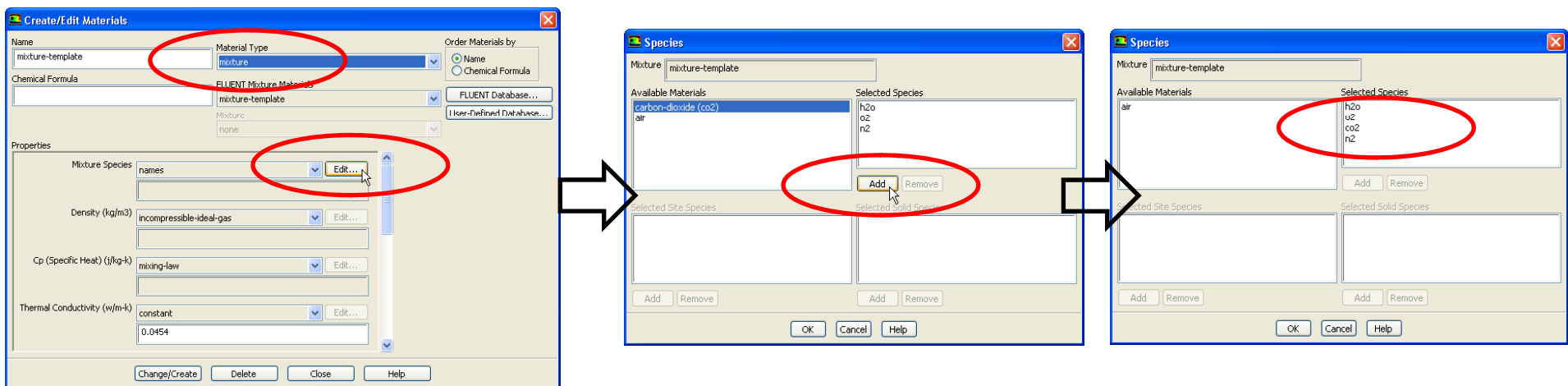
Defining Materials (2)

- Add a mixture species
 - In the Create/Edit Materials panel click on FLUENT Database.
 - The FLUENT Database Materials panel will appear.
 - Select Fluid as Material Type.
 - All predefined fluids materials will be listed under FLUENT Fluid Materials.
 - Select carbon-dioxide (co2).
 - Click Copy.
 - The TUI will inform you that carbon-dioxide has been added.
 - Close the FLUENT Database Materials panel.



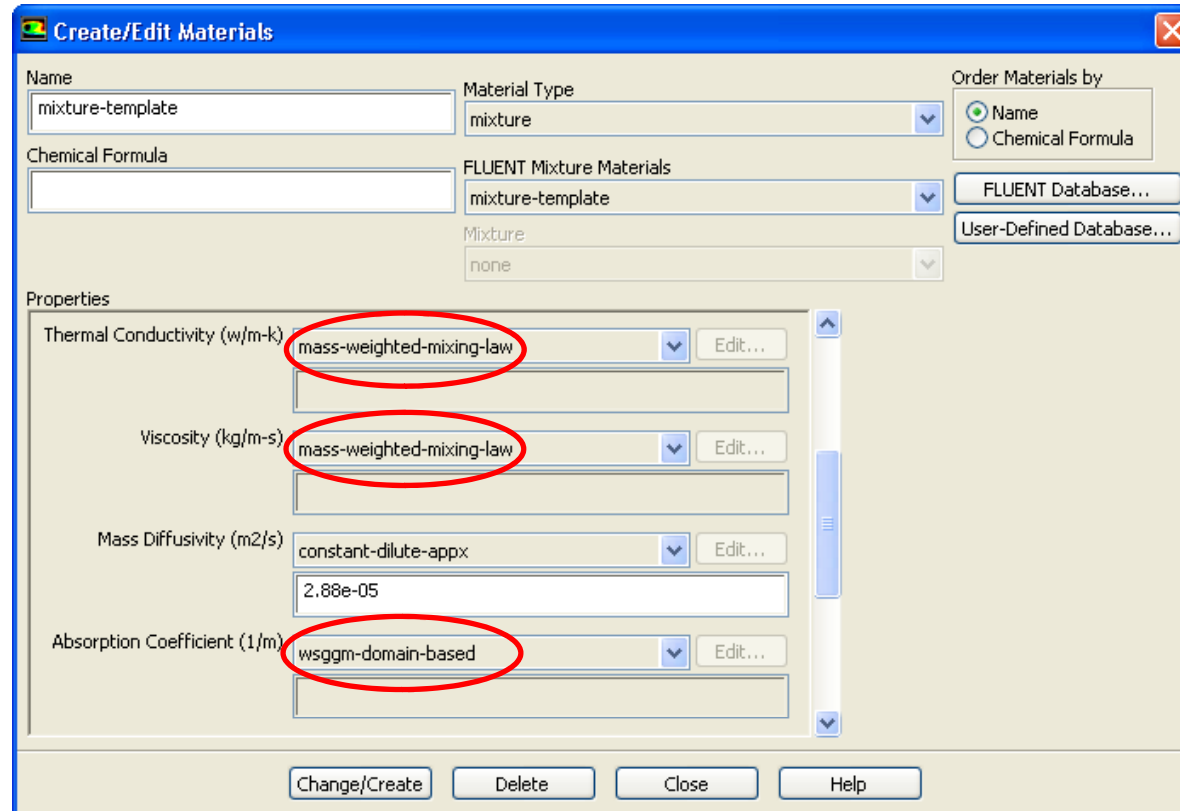
Defining Materials (3)

- Add a mixture species
 - Copying carbon-dioxide(co2) from the fluid database has made the species available to the simulation, now add it to the mixture.
 - In the Create/Edit Materials panel ensure Material Type is set to Mixture and click the Edit button for the Mixture Species.
 - In the Species panel select co2 from the Available Materials list and use the Add button to add it to the Selected Species list. The Selected Species defines the component species of the mixture.
 - The order of the species listed under Selected Species is important. The most abundant species should be listed last. Use the Remove button to remove n2 followed by the Add button to replace n2 as the last species. Click OK.



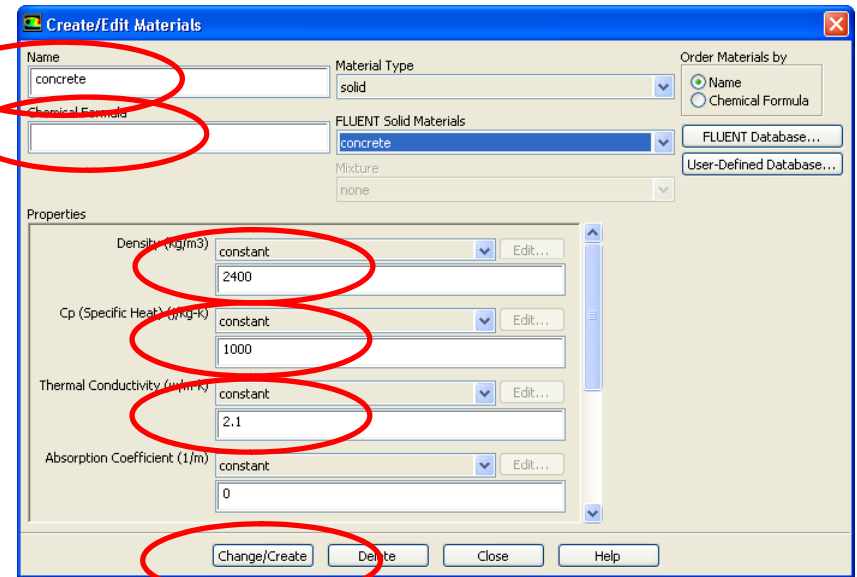
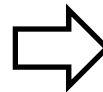
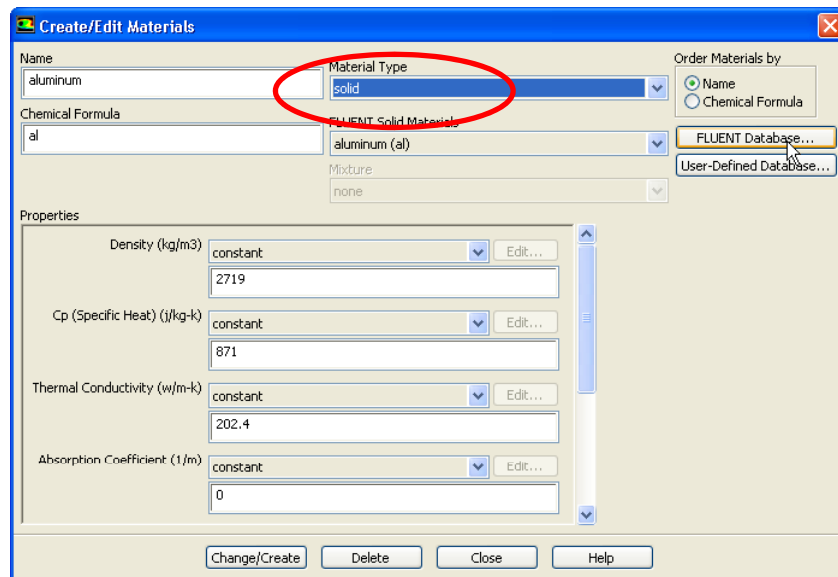
Defining Materials (4)

- Specify mixture
 - Modify the existing settings for Thermal Conductivity, Viscosity and Absorption Coefficient as shown below. Click Change/Create to apply the changes.



Defining Materials (5)

- Specify solid material
 - Select Solid under Material Type (The default solid material is aluminum(al)).
 - Modify aluminum (Name, Chemical Formula & Properties) as shown below.
 - Click Change/Create and choose No for overwriting. Close the Create/Edit Materials panel.
 - Selecting No preserves the original material (aluminum) and adds the new modified material.

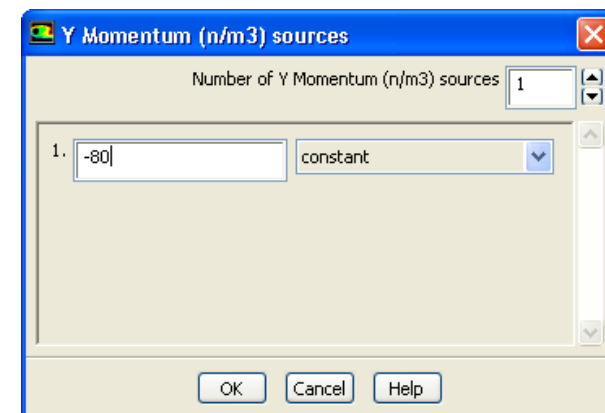
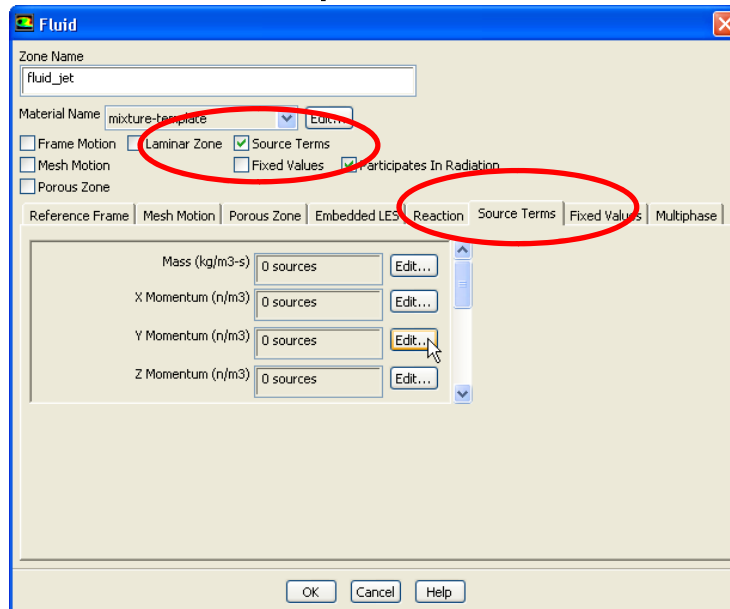


WS3: Modelling Multi Species Flow

Cell Zone Conditions (1)

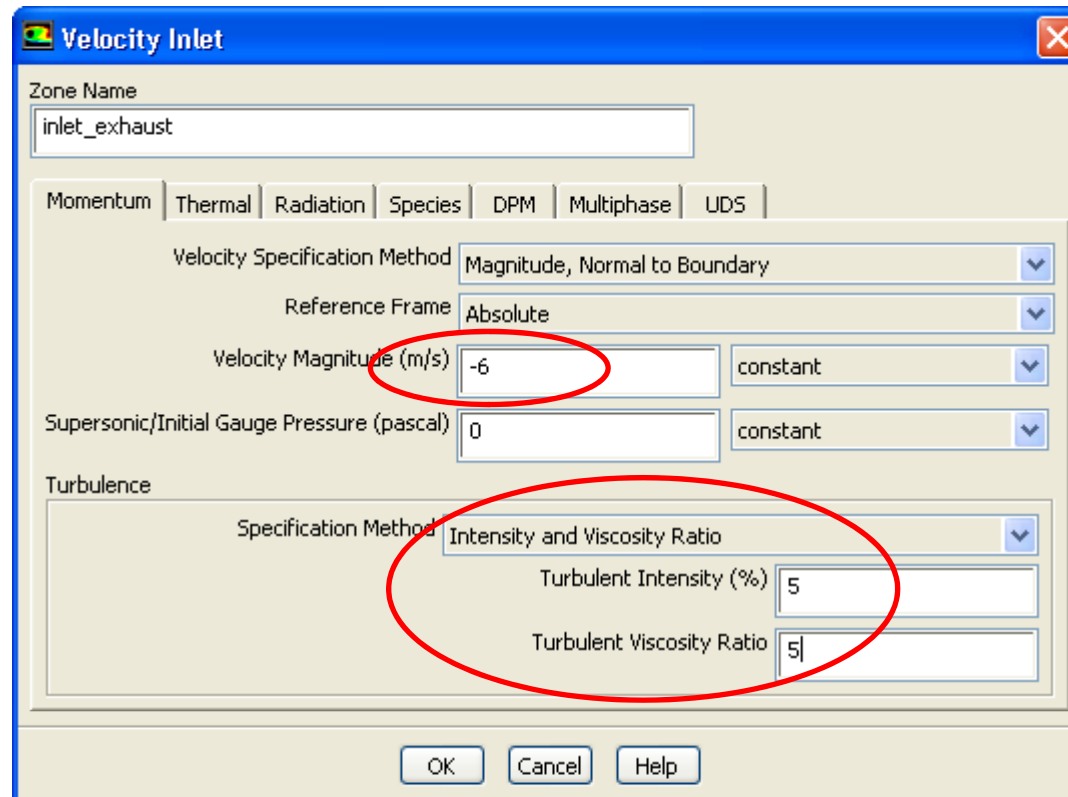


- Set cell zone conditions
 - Select Cell Zone Conditions from the Navigation Pane.
 - Double click fluid_jet from the Zone list.
 - Activate Source Terms.
 - Select the Source Terms tab and click on Edit for Y Momentum.
 - Add 1 source, select Constant and enter a value of -80 (n/m^3)
 - Click OK in both panels.



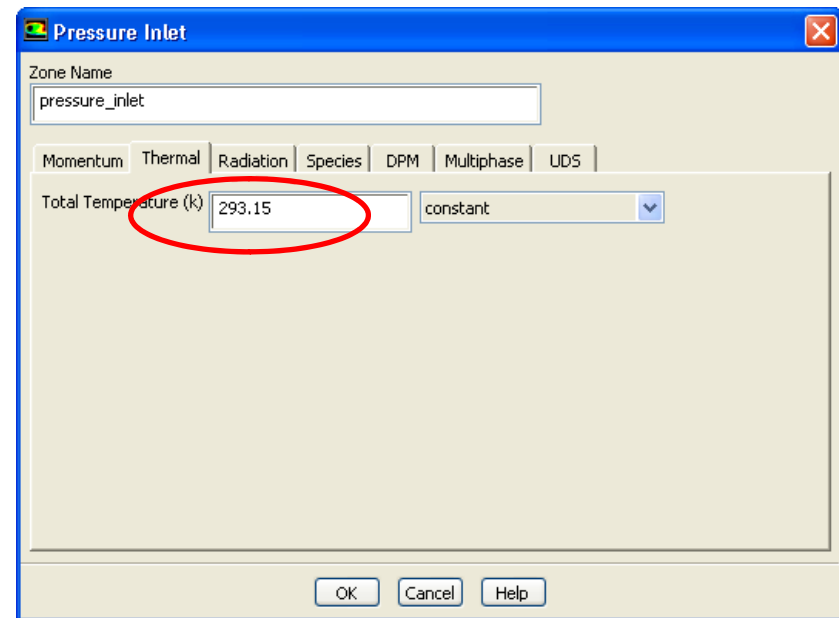
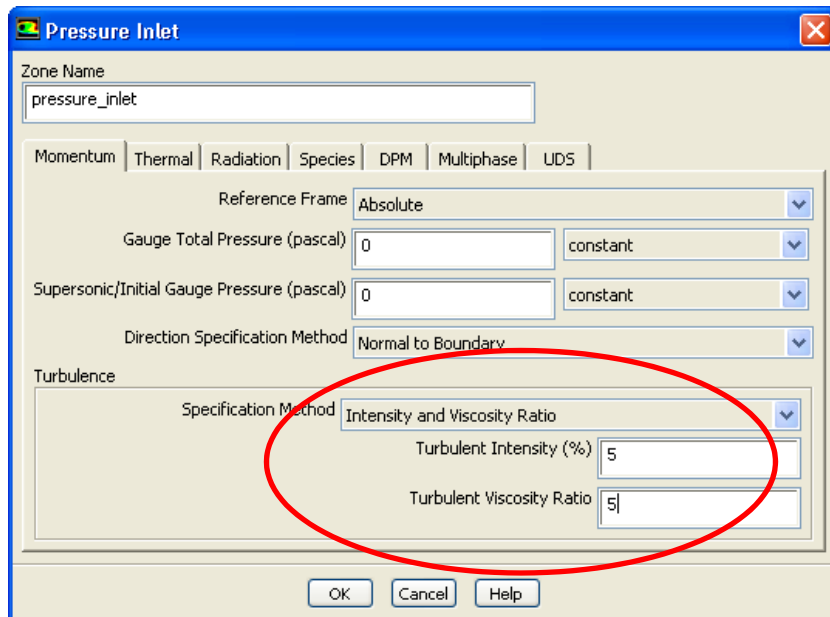
Boundary Conditions (exhaust 1)

- Set boundary conditions
 - Select Boundary Conditions from the Navigation Pane.
 - Double click inlet_exhaust from the Zone list.
 - Apply Momentum settings as shown.
 - Click OK.



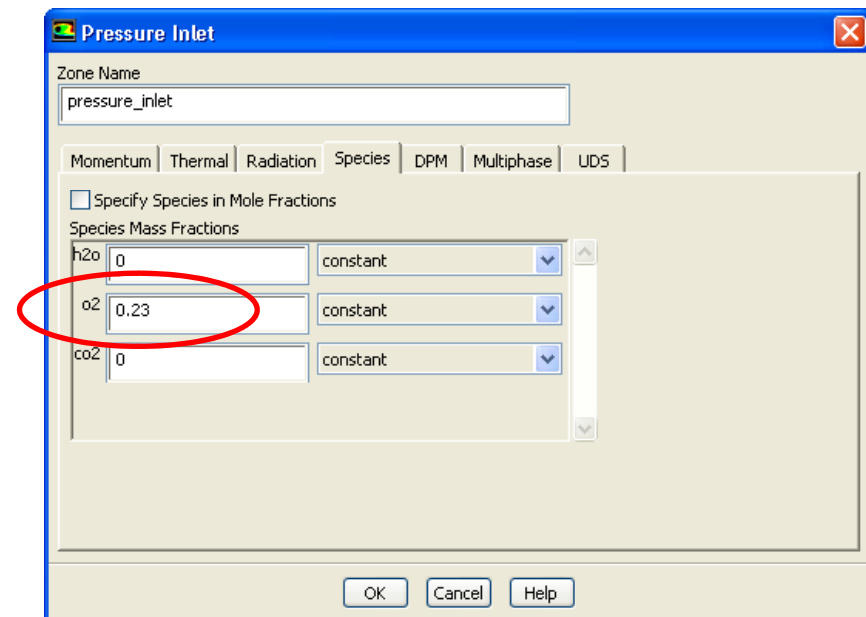
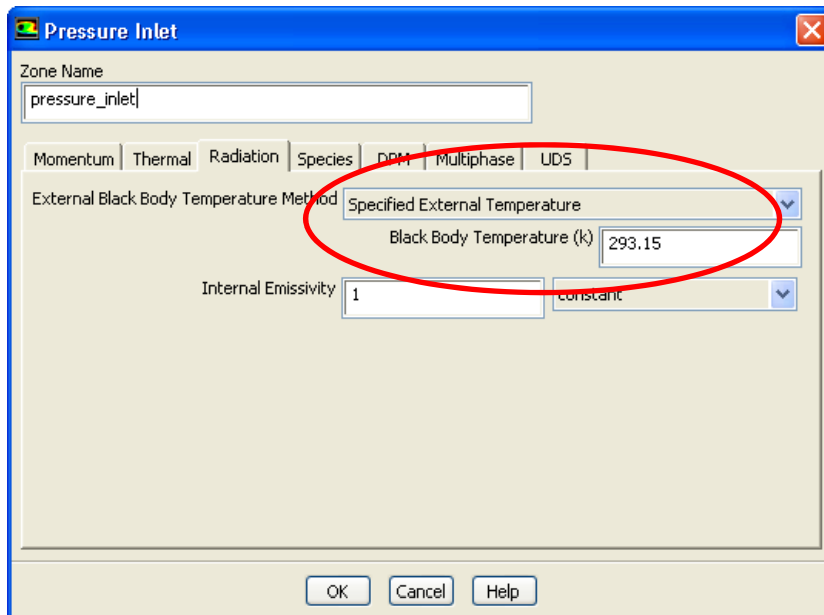
Boundary Conditions (inlet 1)

- Set boundary conditions
 - Double click pressure_inlet from the Zone list.
 - Apply Momentum and Thermal settings as shown.
 - Continued on next page..



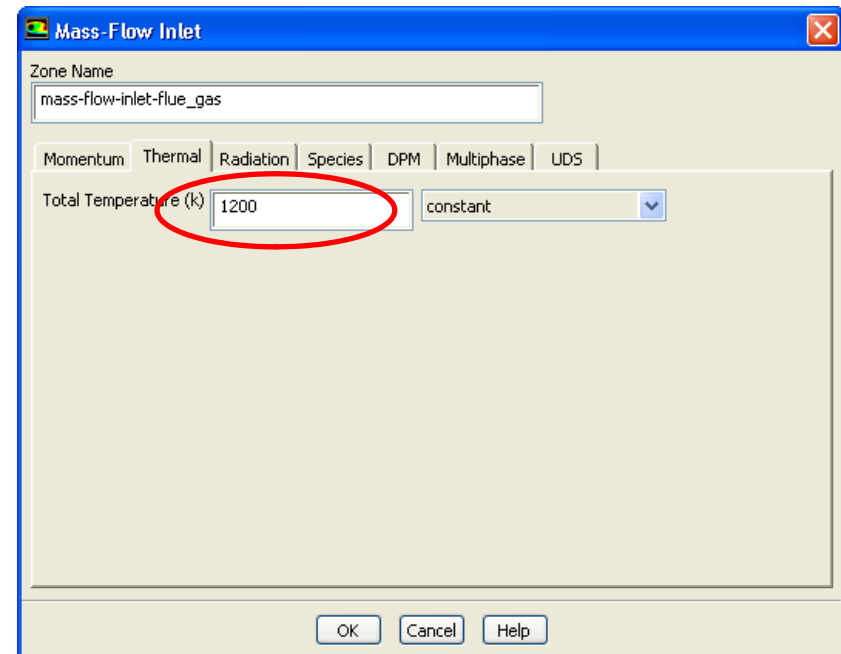
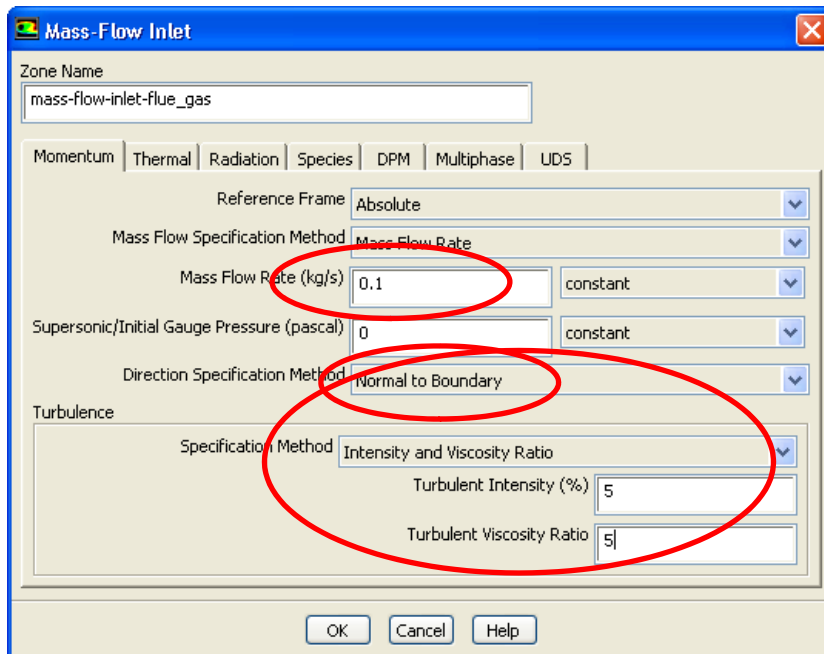
Boundary Conditions (inlet 2)

- Set boundary conditions
 - Apply Radiation and Species settings as shown.
 - Click OK.



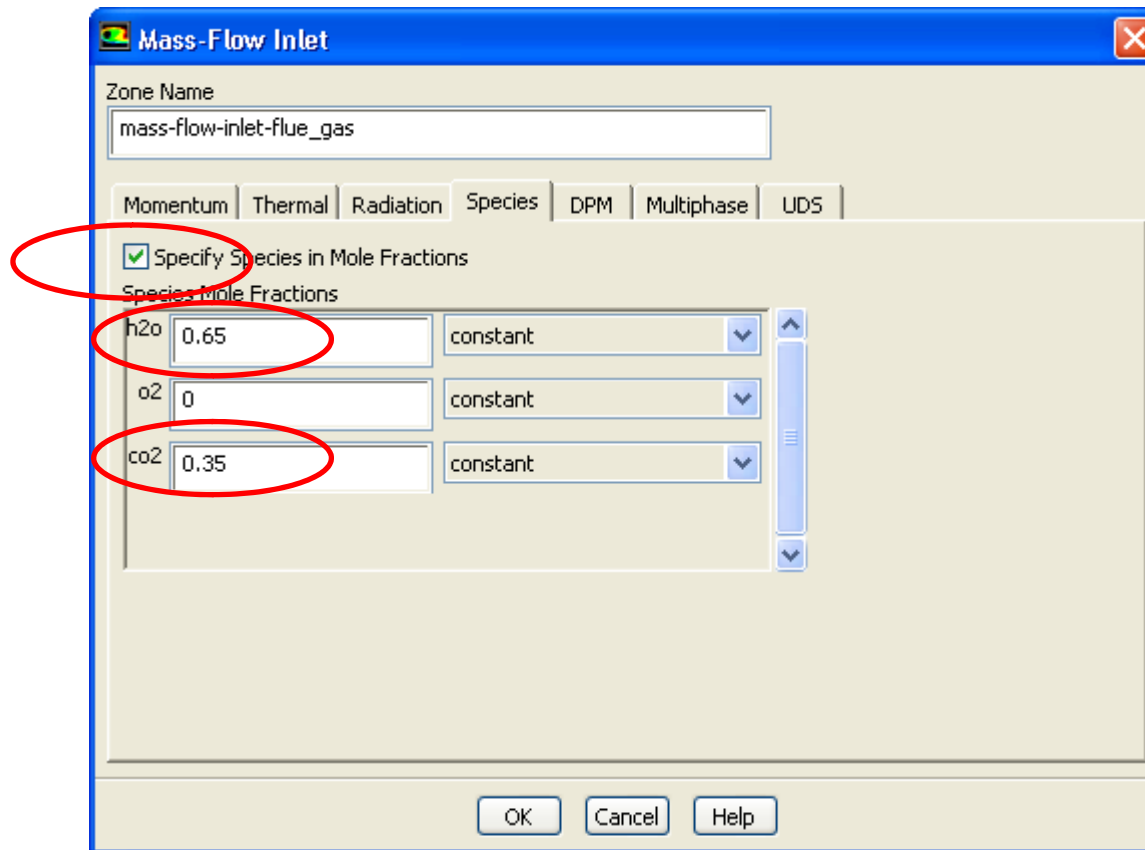
Boundary Conditions (smoke release 1)

- Set boundary conditions
 - Double click mass-flow-inlet-flue_gas from the Zone list.
 - Apply Momentum and Thermal settings as shown.
 - Continued on next page..



Boundary Conditions (smoke release 2)

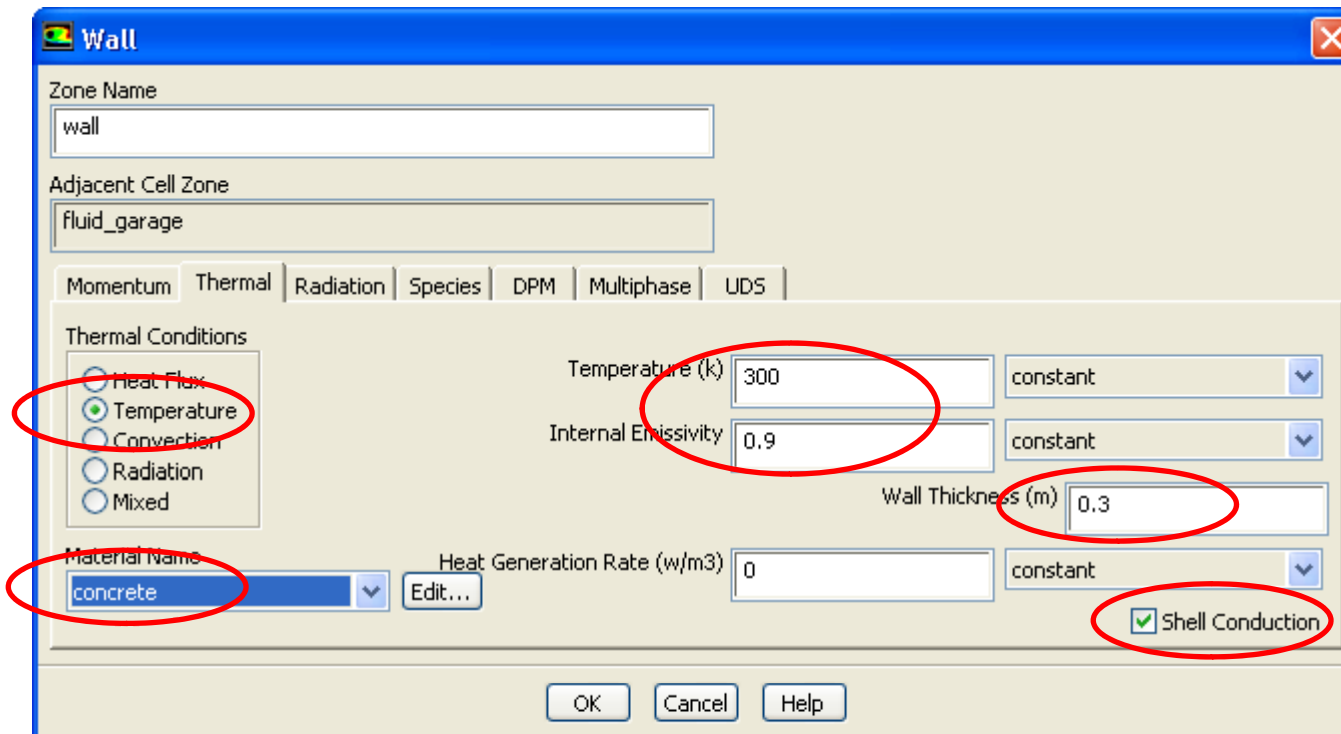
- Set boundary conditions
 - Apply Species settings as shown.
 - Click OK.



Boundary Conditions (walls 1)

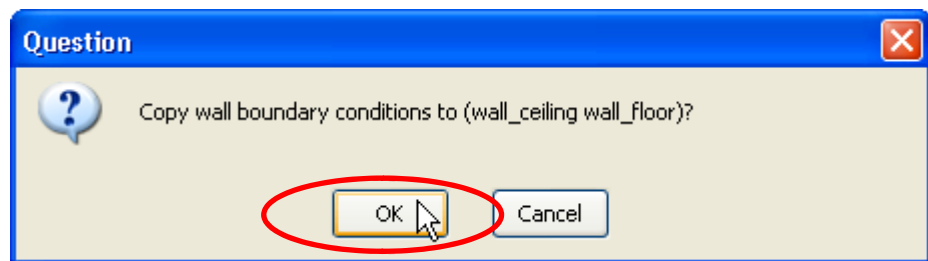
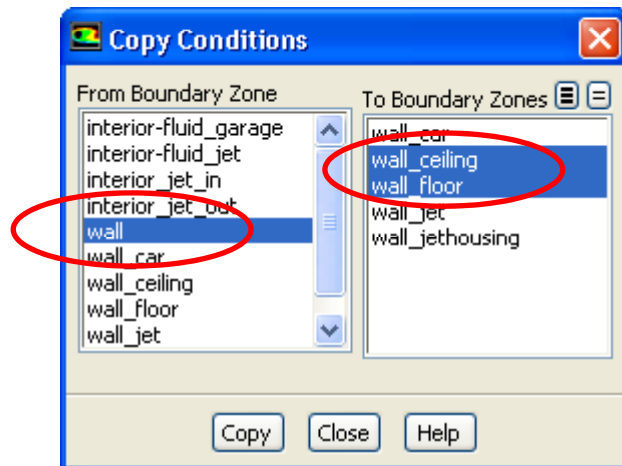
- Set boundary conditions
 - Double click wall from the Zone list.
 - Apply Thermal settings as shown.
 - Click OK.

The Shell Conduction option enables thin walls to solve for heat transfer in both the normal and planar directions without the need to volume mesh them.



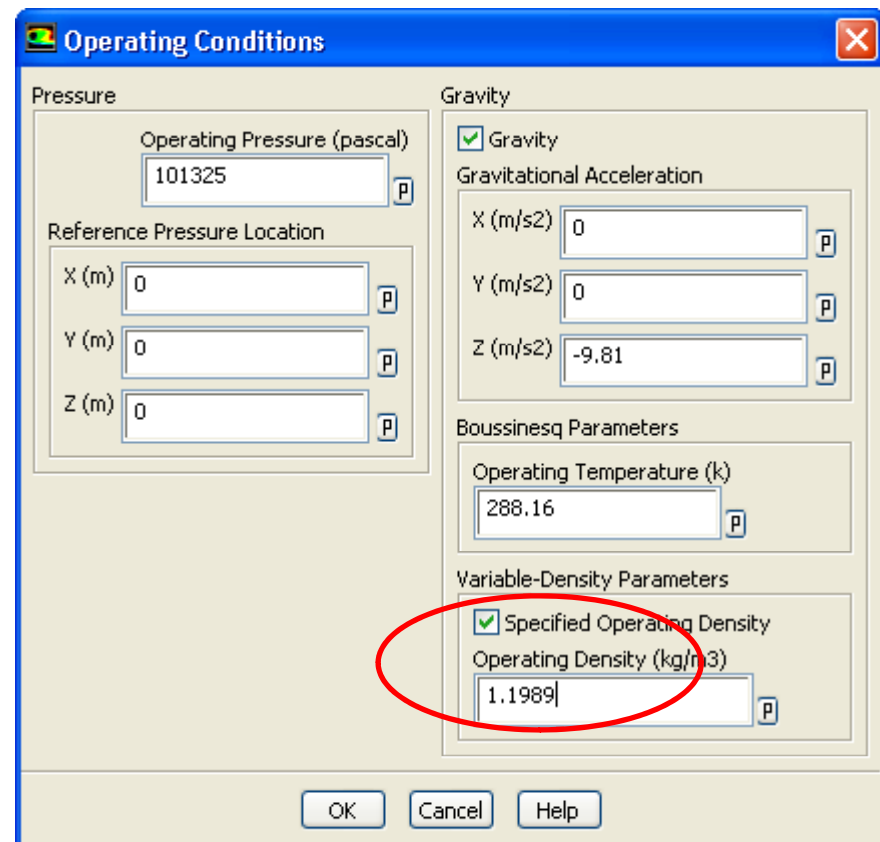
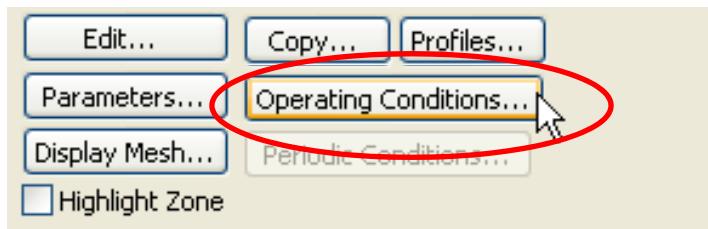
Boundary Conditions (walls 2)

- Set boundary conditions
 - Select Copy from the Boundary Conditions Pane.
 - Select wall in the From Boundary Zone list and wall_ceiling and wall_floor in the To Boundary Zones list.
 - Click Copy, click OK in the question dialog box then Close.
 - This will copy all boundary settings from the boundary zone wall to both wall_ceiling and wall_floor.



Operating Conditions

- Set operating conditions
 - Select Operating Conditions.
 - Apply Specified Operating Density settings as shown.
 - Click OK.

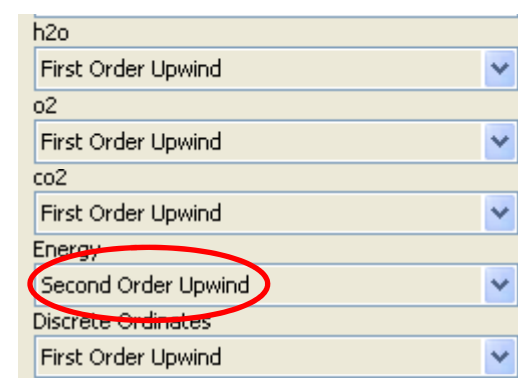
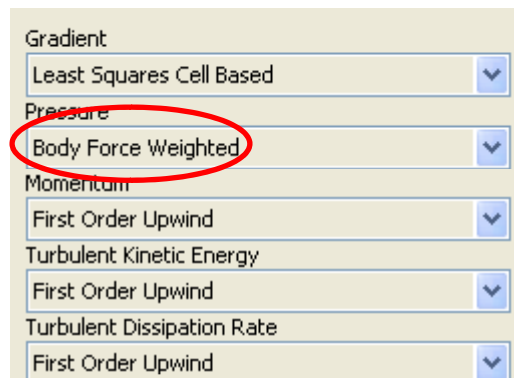


- Notes

- ANSYS FLUENT avoids the problem of roundoff error by subtracting the operating pressure (generally a large pressure roughly equal to the average absolute pressure in the flow) from the absolute pressure, and using the result (termed the gauge pressure). The absolute pressure is simply the sum of the operating pressure and the gauge pressure.
- Operating temperature is only used when using the Boussinesq density model, so in this case, it has no meaning.
- Operating density is also a value for avoiding roundoff errors. For simulations where pressure boundary conditions are present it is important to set the value correctly otherwise the pressure at the boundary will be incorrect and may lead to unphysical flow conditions. Here you have to set it to the density for the conditions at the pressure-inlet - a gas at 293.15 K with 23% O₂ and 67% N₂. You can initialize your flow field with these conditions to get the value for the operating density from the postprocessor (e. g. Reports -> Volume Integral). See the Users Guide “Natural Convection and Buoyancy-Driven Flows” for more details.

- Set solution methods

- Select Solution Methods from the Navigation Pane.
- Under Spatial Discretization set Pressure to Body Force Weighted and Energy to Second Order Upwind.
 - The Body Force Weighted scheme is recommended for problems involving large body forces.
 - The Second Order Upwind scheme is generally recommended for final solutions (first order is less accurate but numerically more stable and is often used for initial approximate solutions).



Solution Controls

- Set solution controls
 - Select Solution Controls from the Navigation Pane.
 - Set Under-Relaxation Factors as listed below.
 - Lower Under-Relaxation Factors will reduce the solution change between iterations leading to more stable convergence though requiring more iterations to reach convergence.
 - Pressure = 0.3
 - Density = 1
 - Body Forces = 1
 - Momentum = 0.7
 - Turbulent Kinetic Energy = 0.5
 - Turbulent Dissipation Rate = 0.5
 - Turbulent Viscosity = 0.7
 - h2o = 1
 - o2 = 1
 - co2 = 1
 - Energy = 1
 - Discrete Ordinates = 1

Solution Controls

Under-Relaxation Factors

Pressure
0.3

Density
1

Body Forces
1

Momentum
0.7

Turbulent Kinetic Energy
0.5

Default

Equations... Limits... Advanced...

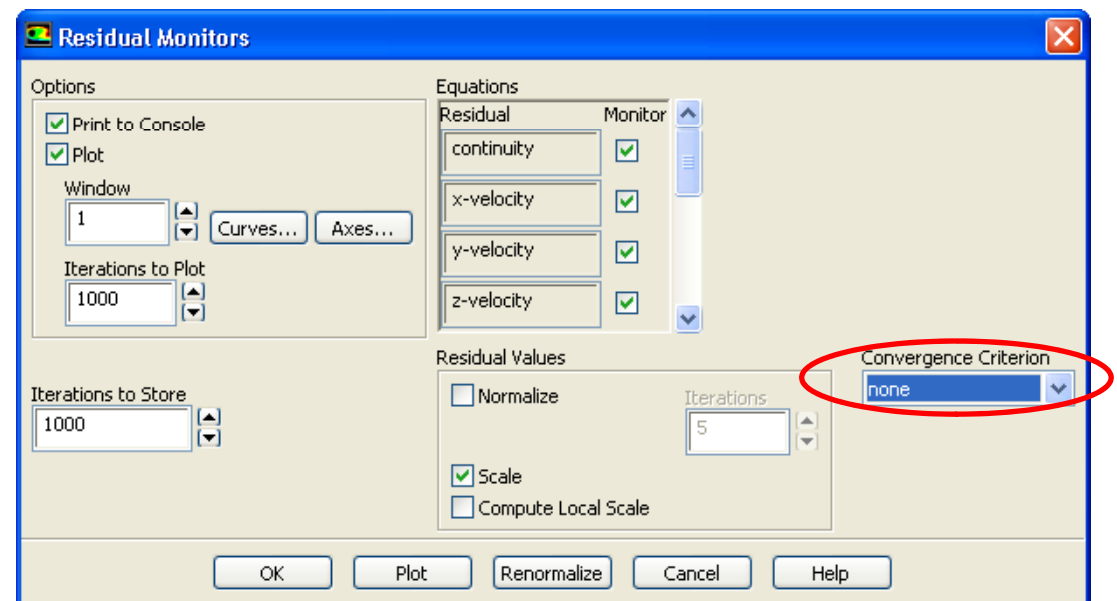
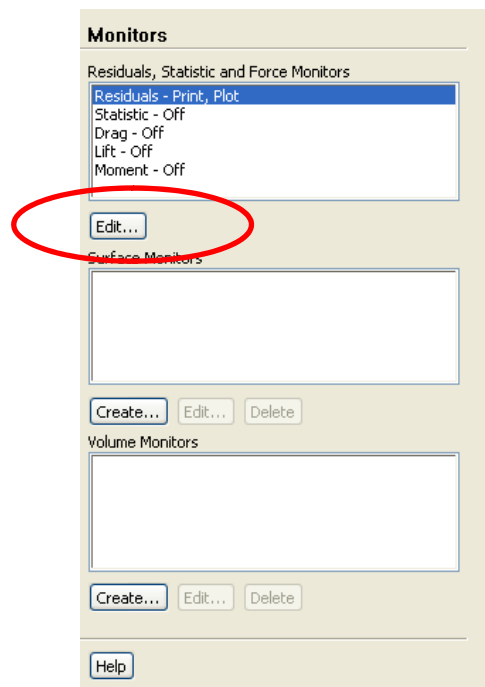
☐ Set All Species URFs Together

Help

Monitors (1)

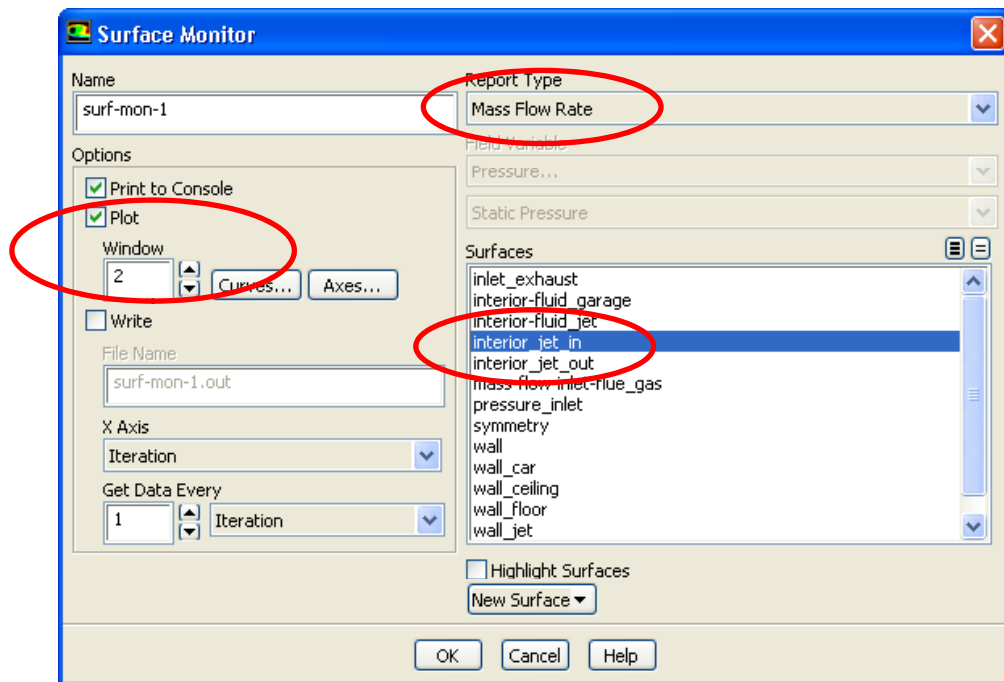
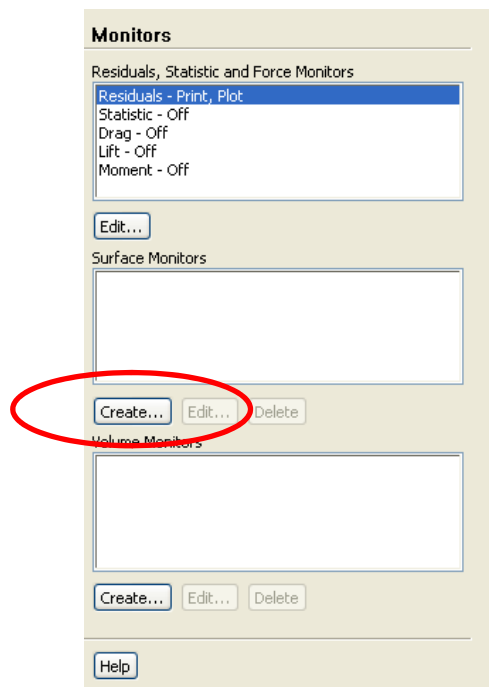
- Set solution monitors

- Select Monitors from the Navigation Pane.
- Click Edit and set the Residual Monitors as shown below.
 - By default ANSYS FLUENT will plot residuals to the window and print to the console. The default setting for the convergence criterion is Absolute which means that the solver will continue until all residuals fall below the Absolute Criteria values specified in the Equations box. Switching the Convergence Criterion to none will cause the solver to continue until a maximum number of iterations is reached. Click OK.



Monitors (2)

- Set surface monitors
 - Under Surface Monitors, click Create.
 - Residuals monitor the numerical accuracy of the solution. However, it is equally important to ensure that solution variables have converged to sensible stable values. Creating Surface Monitors enables solution values of interest to be monitored on specific surfaces within the domain. Here, the mass flow rate will be monitored on the surface “interior_jet_in”. The monitor will be plotted to window 2 and printed to the console.
 - Set the Surface Monitor as shown below and click OK.



Monitors (3)

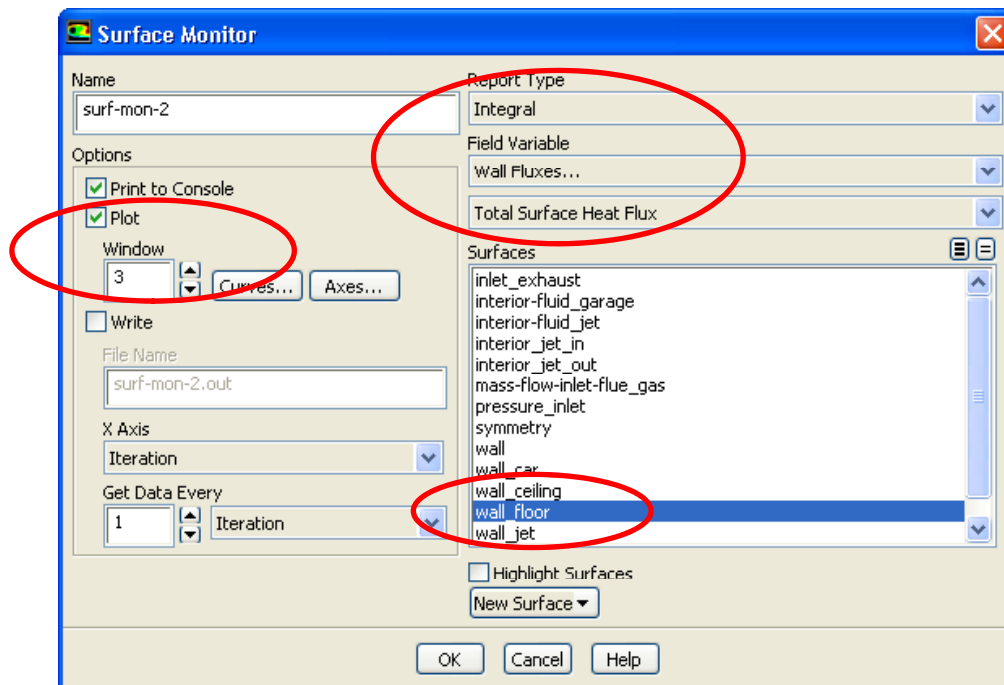
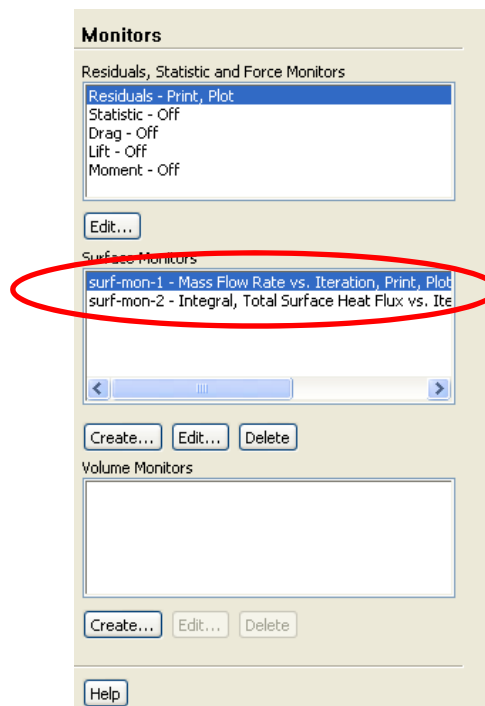
- Set surface monitors

- Create another Surface Monitor.

- There are many different types of calculations that can be performed over surfaces listed under Report Type. This time we will monitor the integral of the Total Surface Heat Flux on the surface “wall_floor” plotting to window 3 and printing to the console.

- Set the Surface Monitor as shown below and click OK.

- Created Surface Monitors are listed after creation.



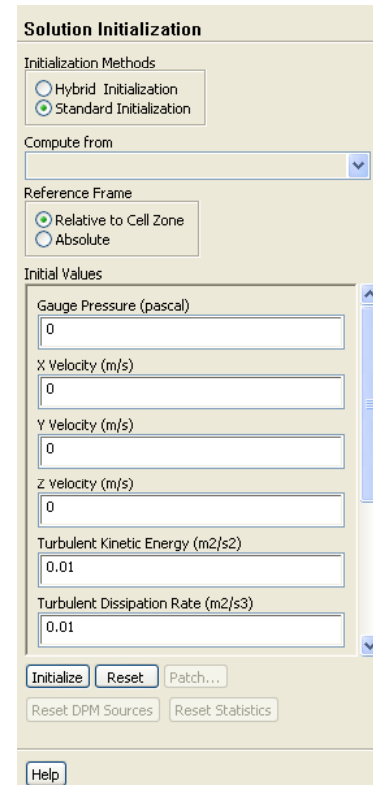
- Notes on monitors

- Buoyancy driven flows often show transient behavior. For this reason, the residuals often will oscillate. Because of this, convergence should always be judged by solution variable monitors and flux reports. The residuals will however show overall for convergence behavior and stability.

In cases of an oscillating steady state solution, a common approach is to continue the simulation in transient mode. In many cases the oscillations will reduce significantly after a few time steps.

The use of surface/volume monitors combined with residuals will provide the best overall judge of solution convergence.

- Set initialization values
 - Select Solution Initialization from the Navigation Pane.
 - The iterative process requires initial values for all solution variables. The default (standard) initialization method applies single values for each variable globally throughout the domain. These values should be within a reasonable range of what is expected in the domain. Specifying unrealistic values could cause convergence problems or require more iterations. Values can be specified manually or can be calculated from any or all boundaries using the Compute from option.
 - Specify the values manually as follows.
 - Initial Values
 - Gauge Pressure = 0
 - X Velocity = 0
 - Y Velocity = 0
 - Z Velocity = 0
 - Turbulent Kinetic Energy = 0.01
 - Turbulent Dissipation Rate = 0.01
 - h2o = 0
 - o2 = 0.23
 - co2 = 0
 - Temperature = 300



Solution Initialization

Initialization Methods

☐ Hybrid Initialization
☒ Standard Initialization

Compute from
All Zones

Reference Frame
☒ Relative to Cell Zone
☐ Absolute

Initial Values

Gauge Pressure (pascal)
0

X Velocity (m/s)
0

Y Velocity (m/s)
0

Z Velocity (m/s)
0

Turbulent Kinetic Energy (m2/s2)
0.01

Turbulent Dissipation Rate (m2/s3)
0.01

Initialize Reset Patch...
Reset DPM Sources Reset Statistics

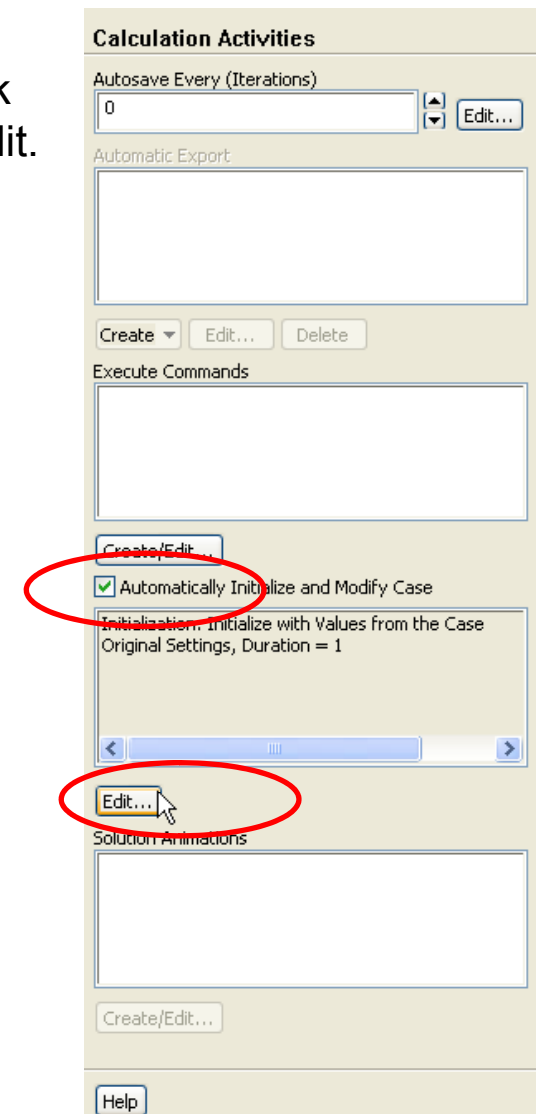
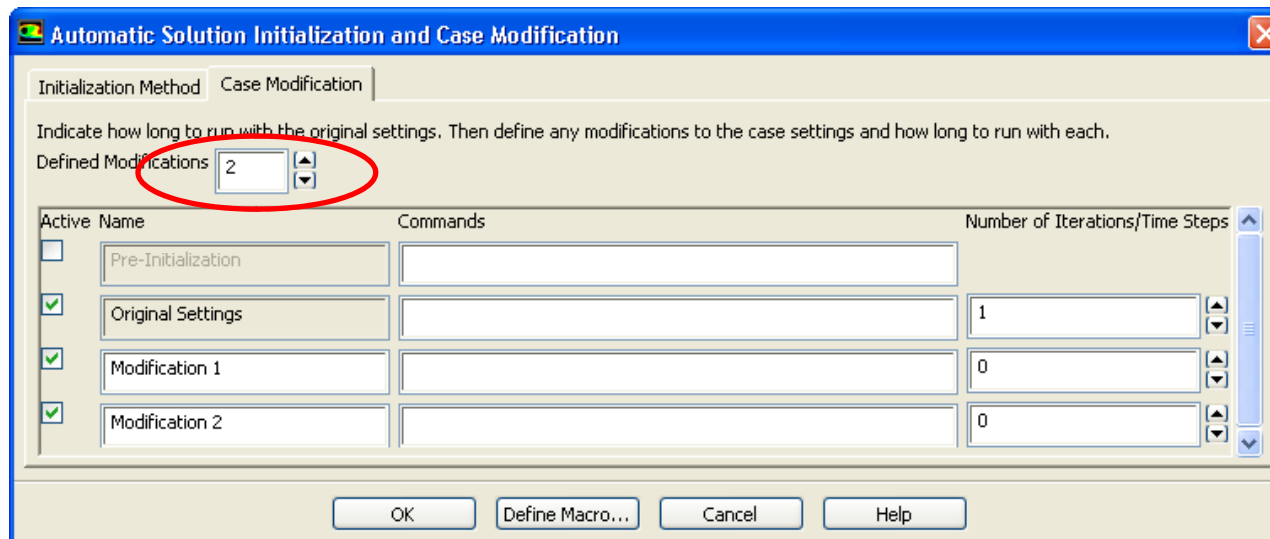
Help

- Changing settings during the calculation
 - Although simulations can often be run to convergence without adjusting the solver controls it is often beneficial to change these settings during the calculation. For example, some equations may not need as many iterations to converge. Also, in many thermal cases, it is advantageous in terms of solution stability to solve the momentum equations first before switching on the energy equation. This step illustrates how to use the Case Modification panel to adjust solver settings during a calculation.
 - In this case we will first solve the full equation set for a small number of iterations, then only solve for mass/momentum before finally solving the full set again.

WS3: Modelling Multi Species Flow

Calculation Activities (2)

- Changing settings during the calculation
 - Select Calculation Activities from the Navigation Pane, check the Automatically Initialize and Modify Case box and click Edit.
 - Select the Case Modification tab.
 - Using the defaults would result in the simulation being run using the existing settings ('Original Settings') for 1 iteration.
 - We will be running using the original settings then apply 2 modifications. Increase Defined Modifications to 2.



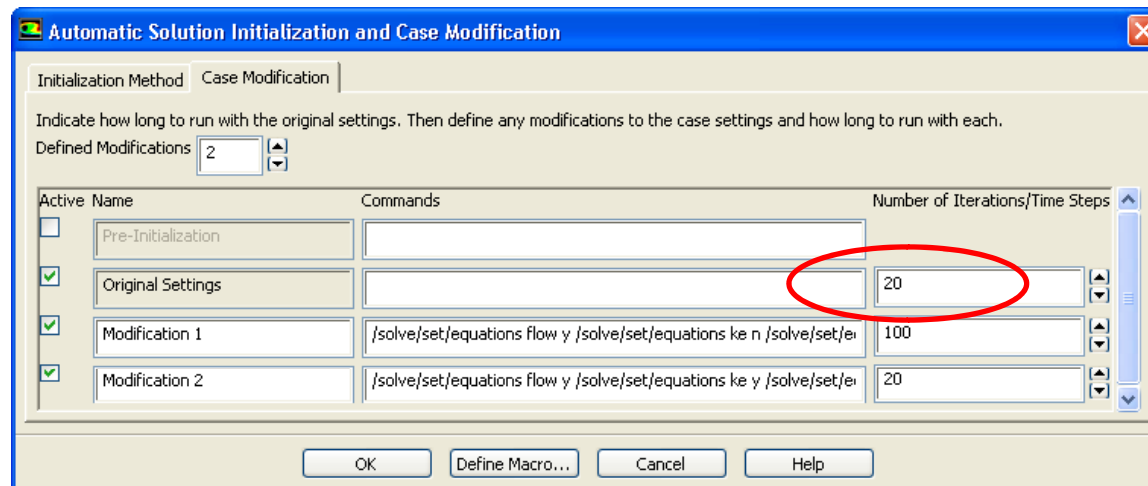
WS3: Modelling Multi Species Flow

Calculation Activities (3)



- Changing settings during the calculation

- Commands are entered using the Text User Interface (TUI) syntax. Options selected using the Graphical User Interface (GUI) have equivalent TUI commands.
- Rather than type these out a journal file is provided for this workshop that will enter these for you.
- From the main menu, File>Read>Journal, Select the journal file “calc_activities.jou” from the user_files directory. Answer No to the question dialog box asking if there are any read/write commands in the journal.
- Modification 1 will switch off all equations except the flow equations and run for 100 iterations.
- Modification 2 will switch all equations back on and run for 20 iterations.
- Set the Number of Iterations for Original Settings to 20.
- Click OK and answer No to the question dialog box.

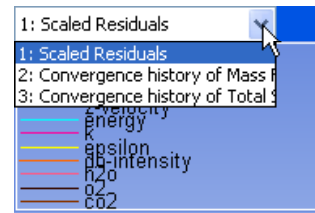
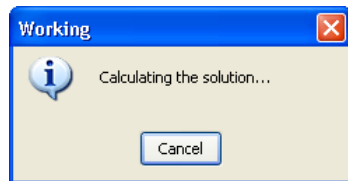
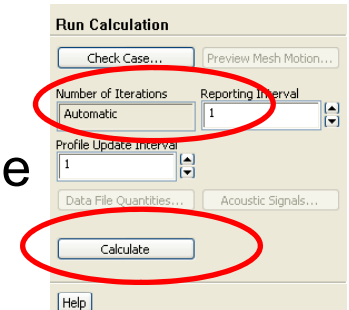


- Changing settings during the calculation
 - The modifications now contain the TUI commands for switching various equations on and off.
 - For example, the TUI command for switching off the energy equation is of the form; (substituting n for y to switch on)
 - **/solve/set/equations temperature n**
 - The list of available TUI commands is extensive and goes beyond options available in the GUI.
 - All aspects of the solver can be controlled using TUI commands.
 - The journal used here contained the TUI commands to setup up the 2 case modifications.
 - Consult the documentation for a more comprehensive description of TUI command usage.

Run Calculation

- Start the calculation

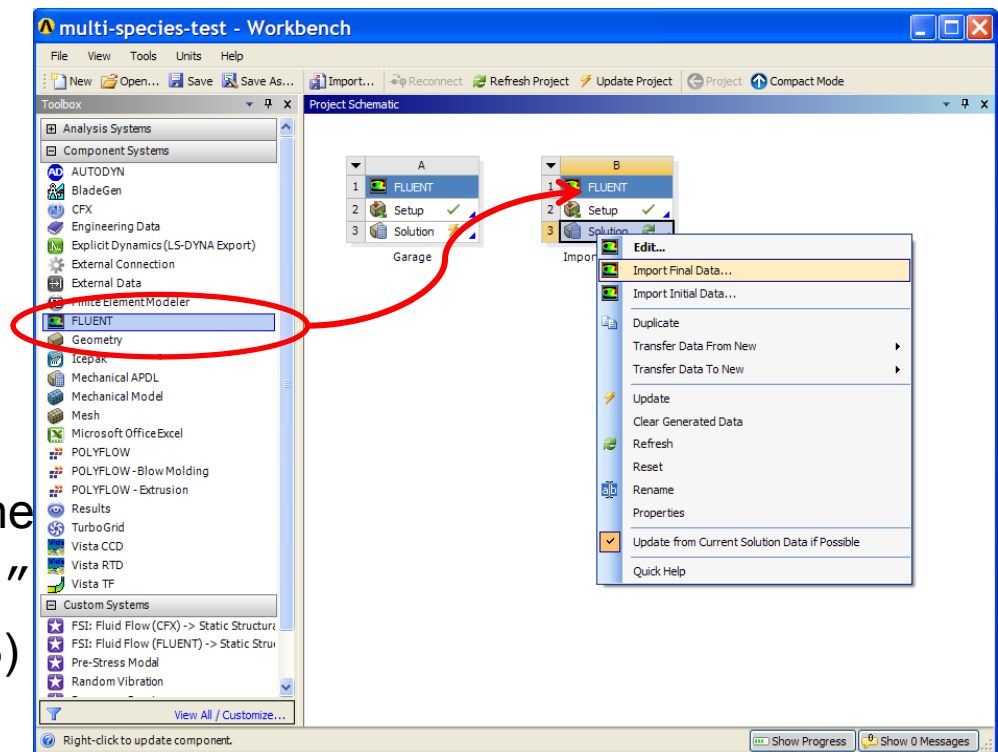
- Select Run Calculation from the Navigation Pane.
 - The Number of Iterations is set to Automatic since this has been defined in the Case Modification panel.
- Before starting the calculation it is good practice to save the project.
 - File>Save Project.
- The calculation will take approximately 40 minutes in serial.



- However if you are short of time, we have supplied a converged model that you can use instead (see next slide).

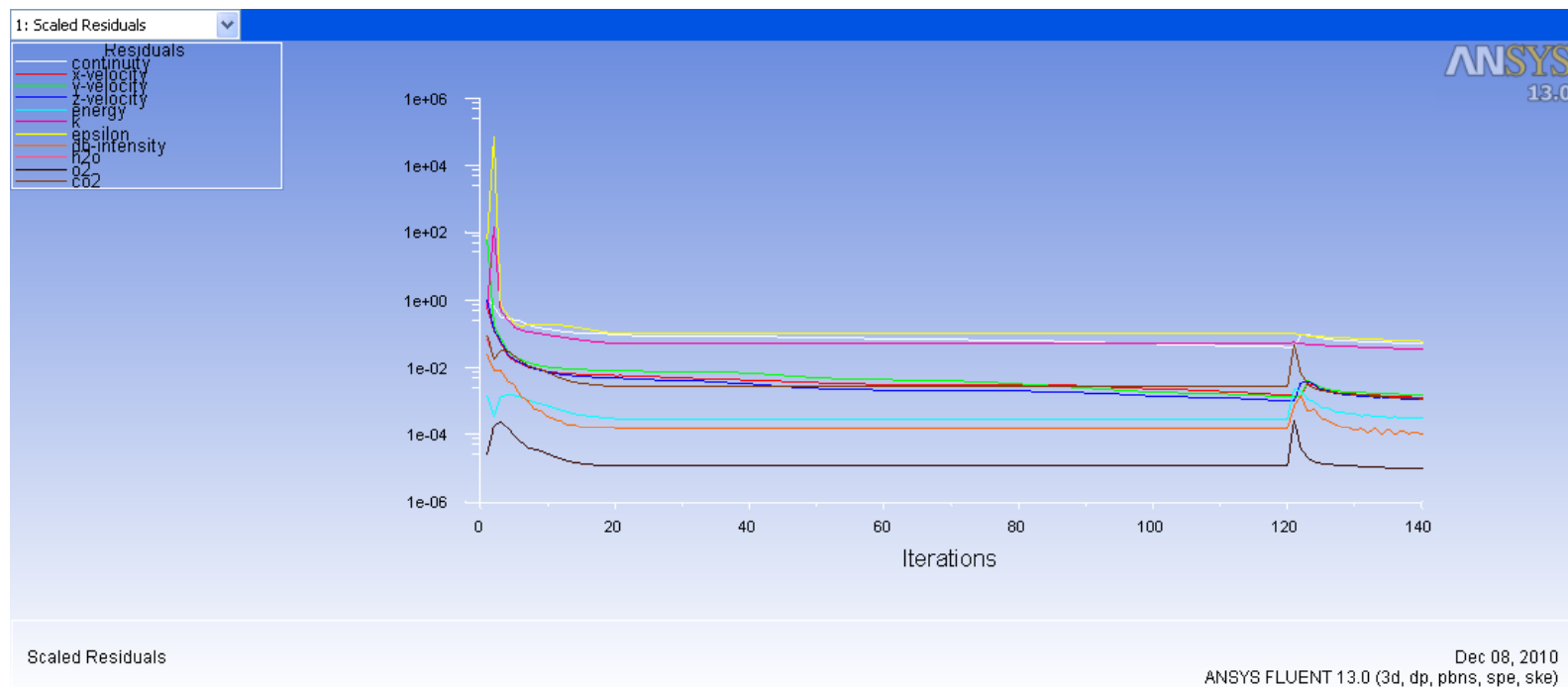
There are times when you may want to bring a solution (perhaps made on a remote cluster) into your workbench session.

1. Stop the iterations. Close the existing FLUENT session, and return to Workbench
2. Drag a new FLUENT session into the Workbench page. Rename as “Imported_Result”.
3. In the Setup Cell (B2), right click and select “Import FLUENT case”
Pick the file “workshop3-converged.cas.gz”
4. FLUENT will start up – **be sure to select double precision**. Once open, close this session again.
5. In the Solution cell (B3), right click and “Import Final Data”, selecting the file “workshop3-converged.dat.gz”
6. Double click on the solution cell (B3) and continue with this workshop.



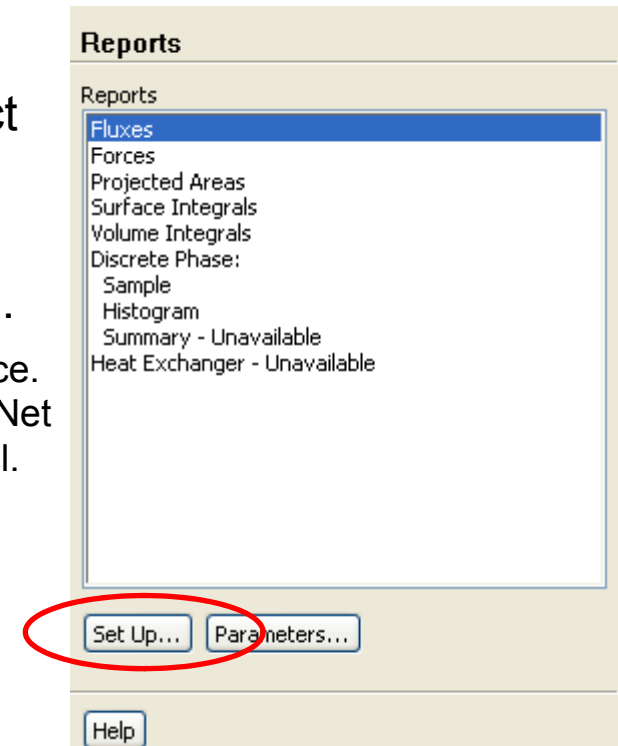
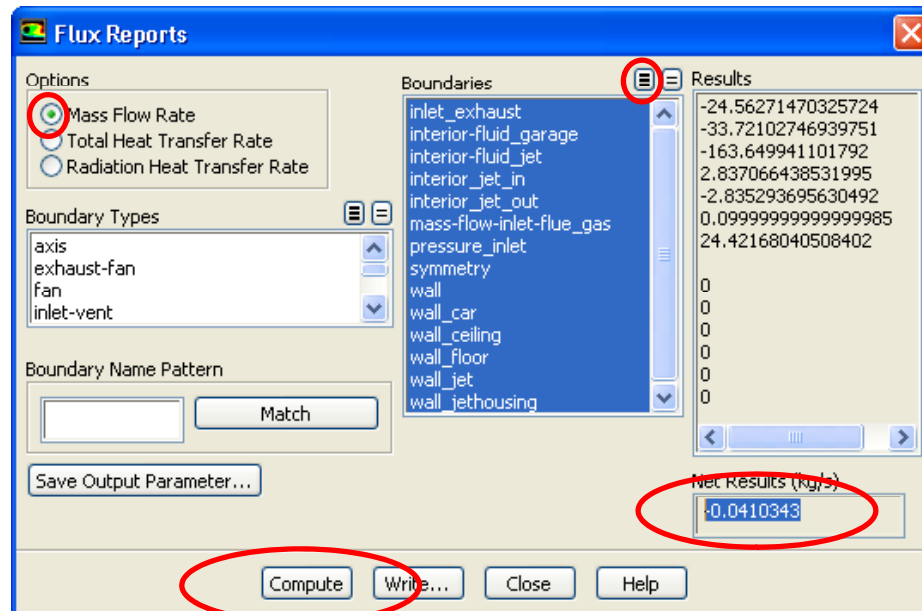
Check Residuals and Monitors (1)

- Check Monitors, Residuals and Fluxes
 - *If progressing from the pre solved project select Monitors from the Navigation Pane, click Edit under Residuals, Statistics and Force Monitors and click Plot in the Residual Monitors Panel that appears.*
 - The residuals are still quite high after 140 iterations and the surface monitors are still changing.



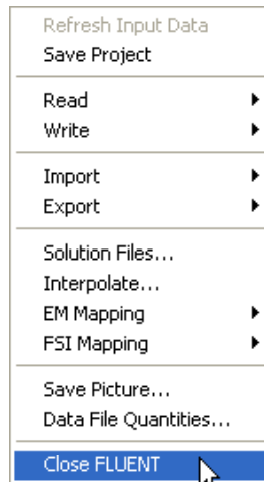
Check Residuals and Monitors (2)

- Check Monitors, Residuals and Fluxes
 - Select Reports from the Navigation Pane and select Fluxes under Reports. Click Setup.
 - In the Flux Reports panel check the Mass balance over all boundaries as shown below. Click compute.
 - Note that the Net Results indicate a relatively large imbalance. This is an indication that the solution is not fully converged. Net heat flux can be calculated in the same way. Close the panel.



- Close Fluent

- Close ANSYS FLUENT by selecting File>Close FLUENT

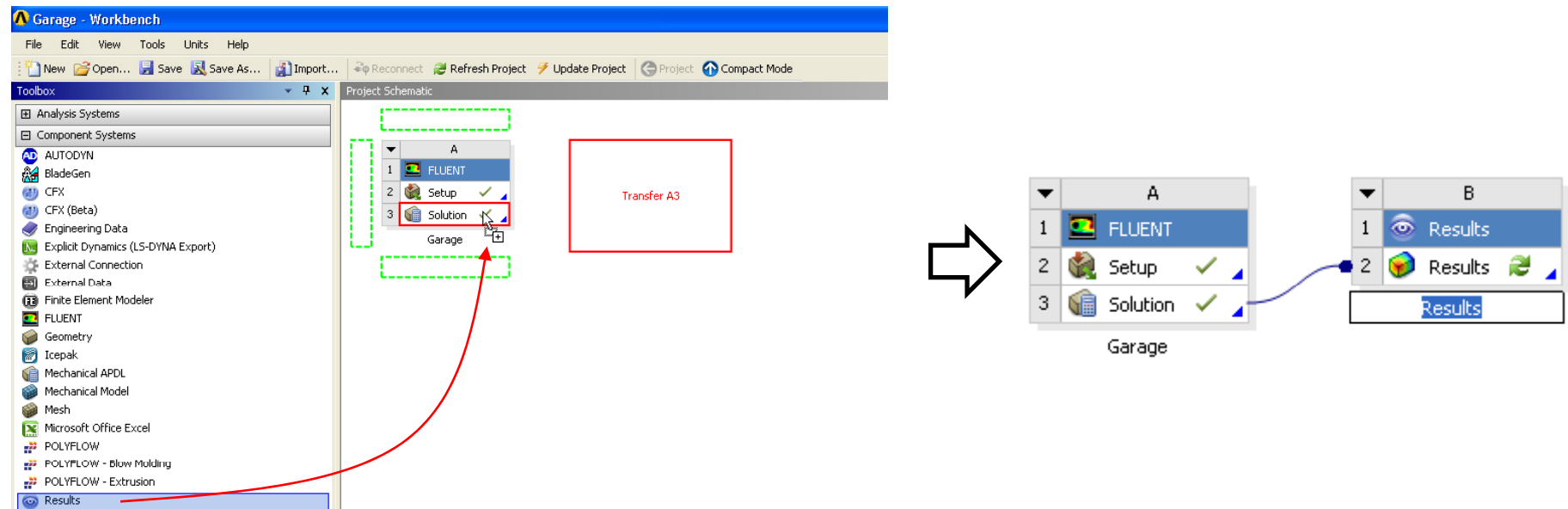


- ANSYS FLUENT contains basic built in post processing capabilities which can be used to quickly assess results graphically and numerically during and after the solution.
- CFD POST is a powerful separate post processing application containing many more advanced features. The remainder of this workshop will introduce some features of CFD POST.

Starting CFD POST

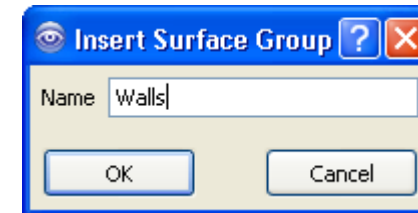
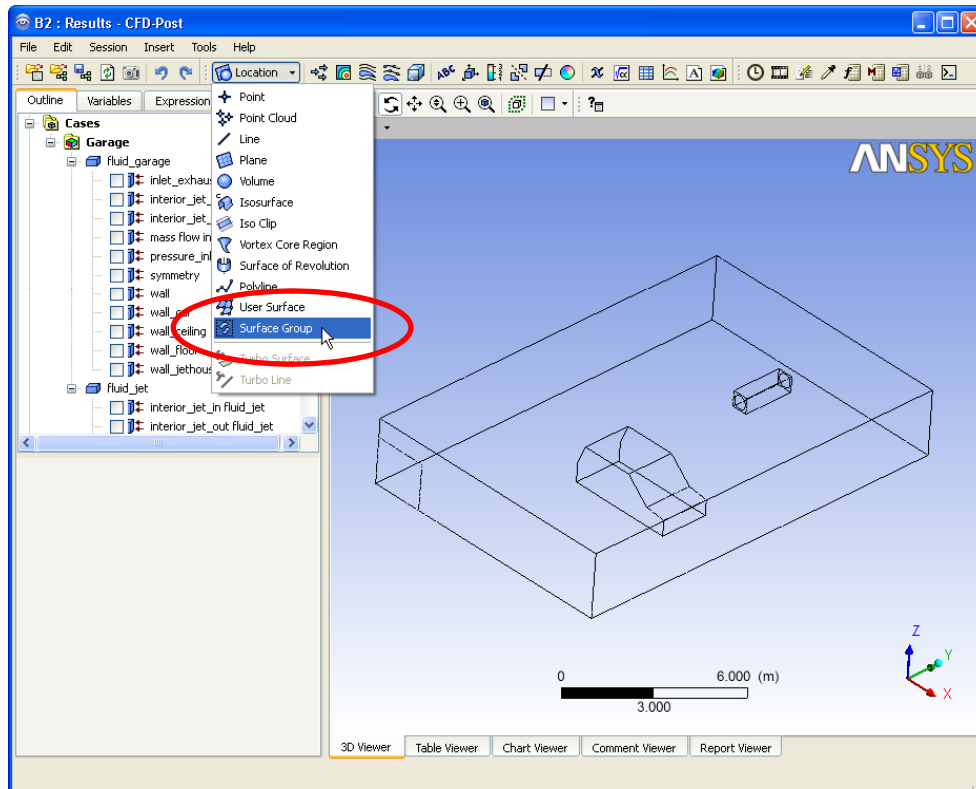
- Add a Results System

- Drag a Results System onto the Solution cell of the FLUENT system.
- This will link a CFD POST (Results) system to the FLUENT system solution data as shown.
- Start CFD POST by double clicking on cell B2.
 - This will start CFD POST and load the FLUENT solution data.

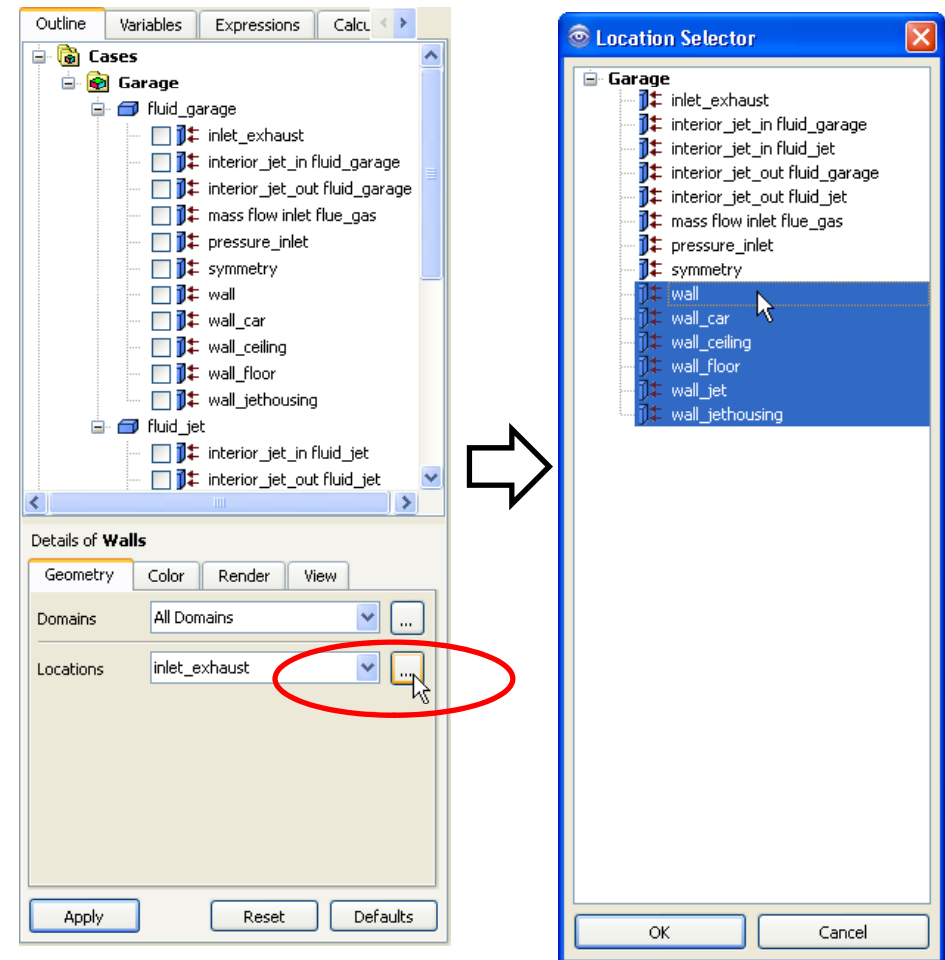


Post Processing – Wall Temperature (1)

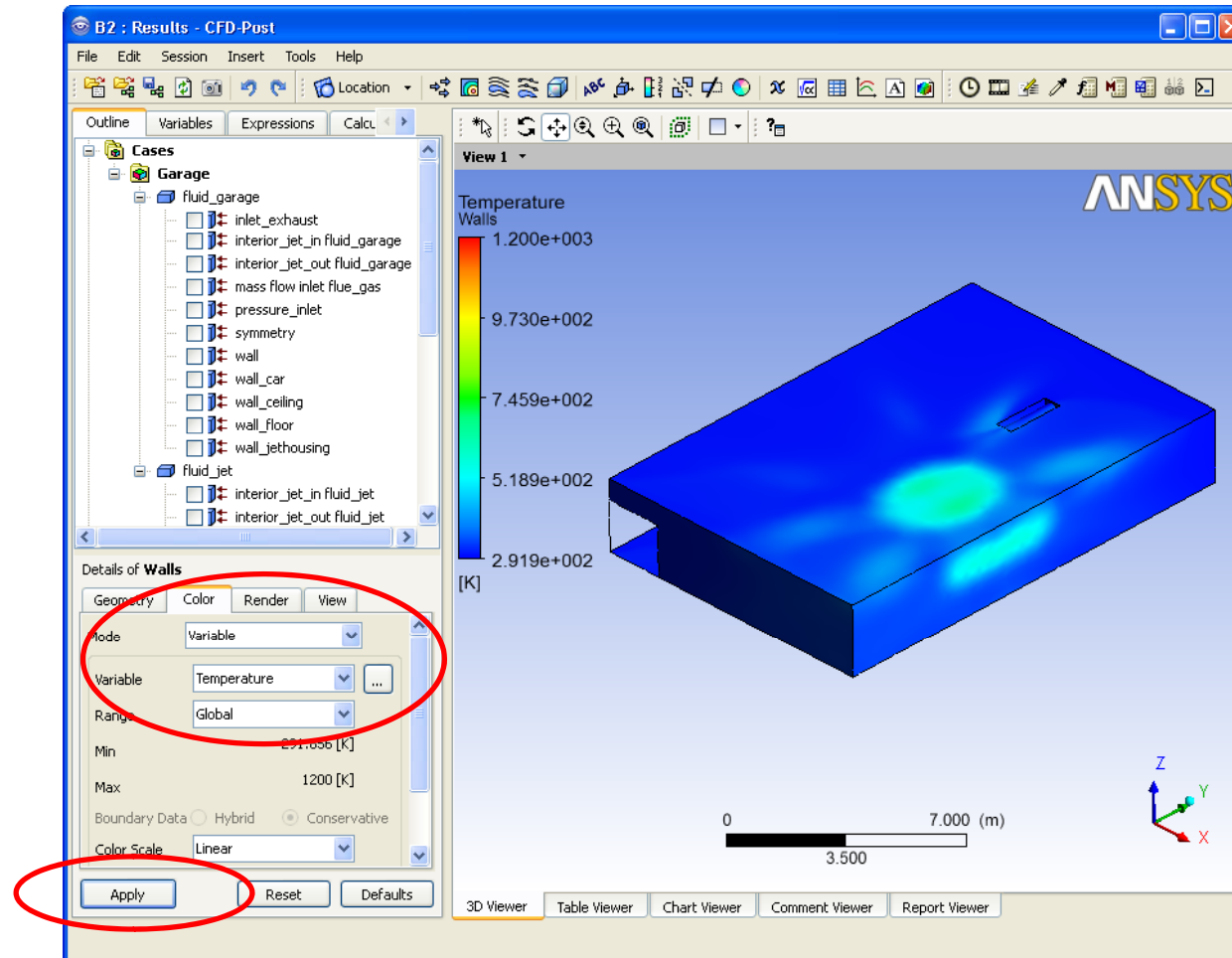
- Add a Location representing a group of surfaces
 - For displaying the temperature on all walls the most effective way is to use a surface group.
 - Select Locations > Surface Group, enter a name as shown below and click OK.



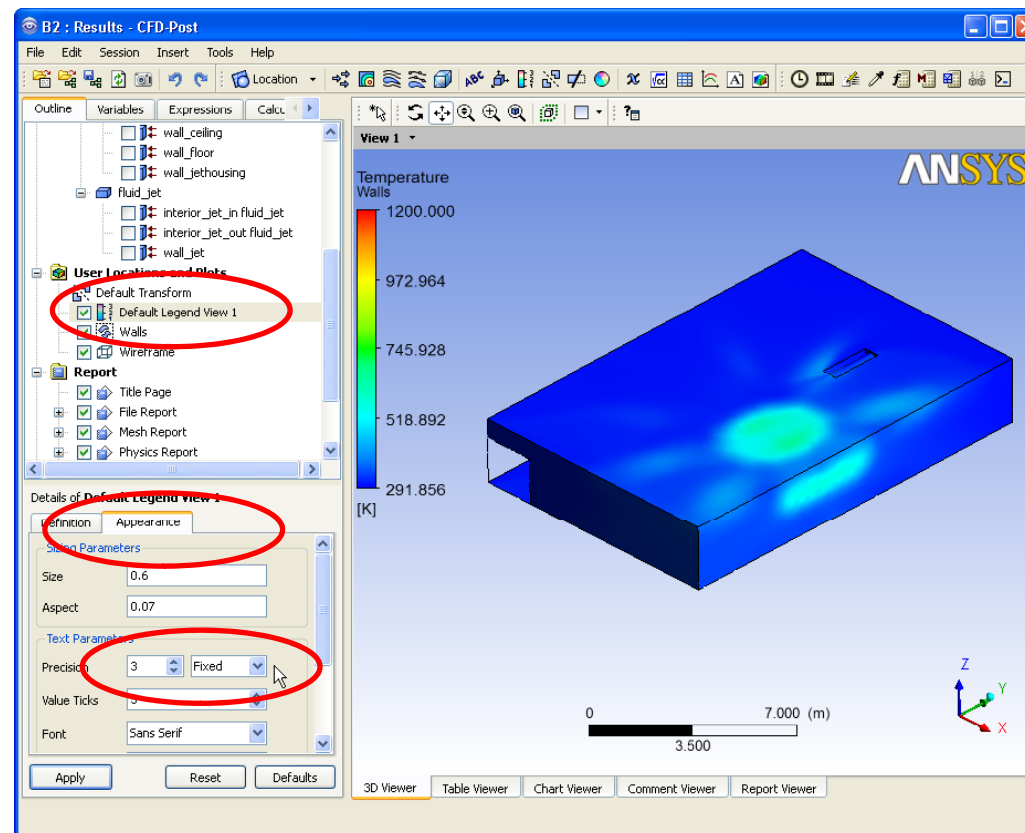
- Define Location details
 - The details of the new location will be displayed in the bottom left pane.
 - Select Locations, click on “...” and select all walls (CTRL click to multiple select).
 - Click OK in the Location Selector.



- Apply contour to Location
 - Select the Color tab, click on Mode and select Variable Temperature and click on Apply.

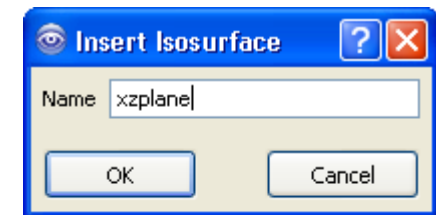
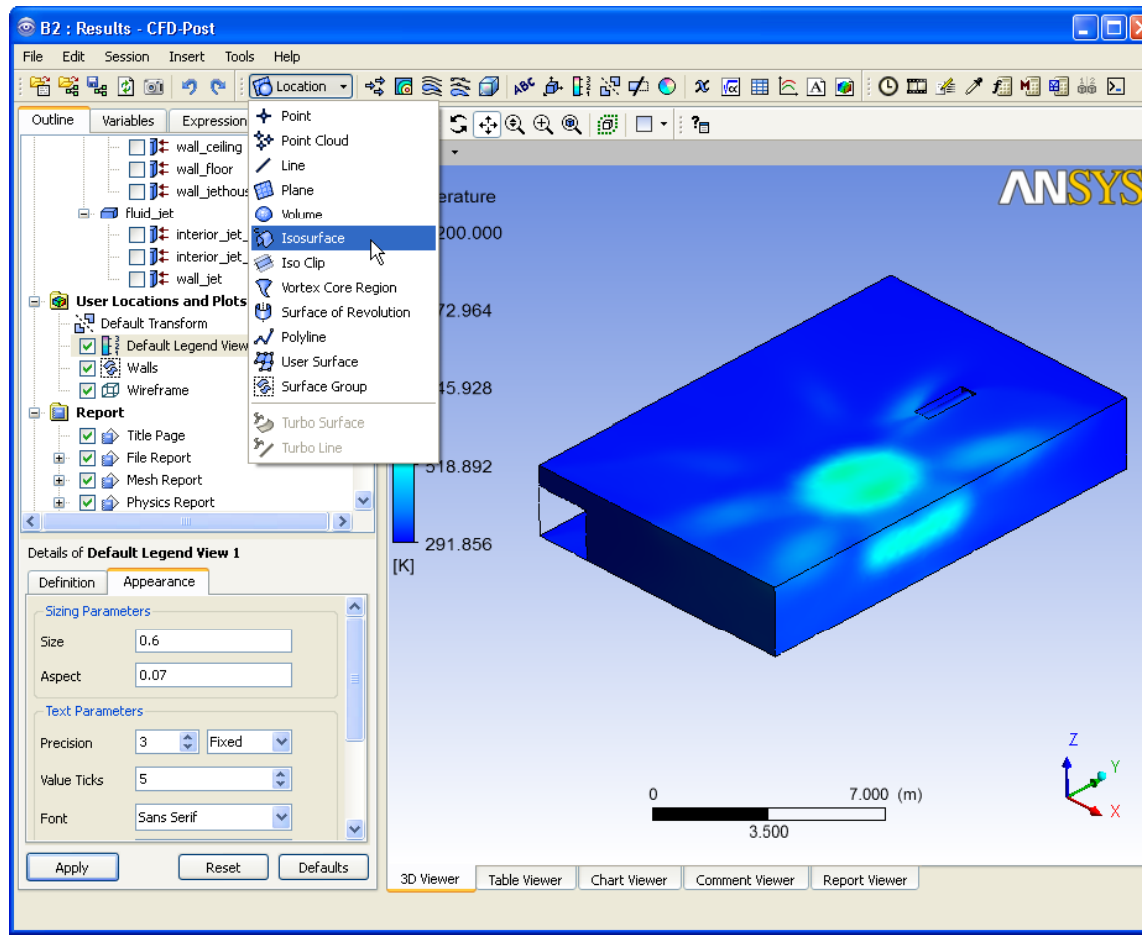


- Make changes to the legend
 - If you want to change the appearance of the legend, select it in the tree (double click) and change the details accordingly – for example, set Precision to Fixed instead of Scientific.



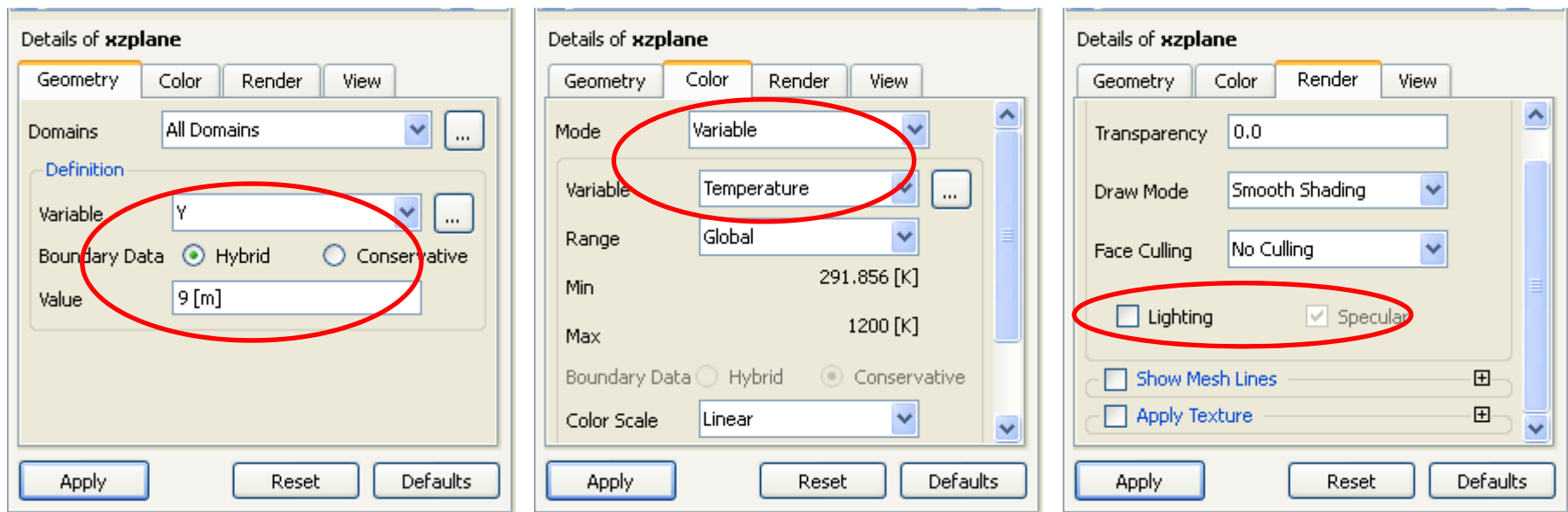
Postprocessing – Section Plane (1)

- Add a Location representing a section plane
 - Select Locations > Isosurface, enter a name as shown below and click OK.

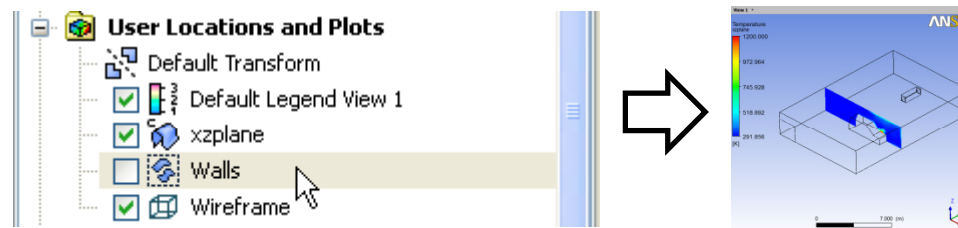


Postprocessing – Section Plane (2)

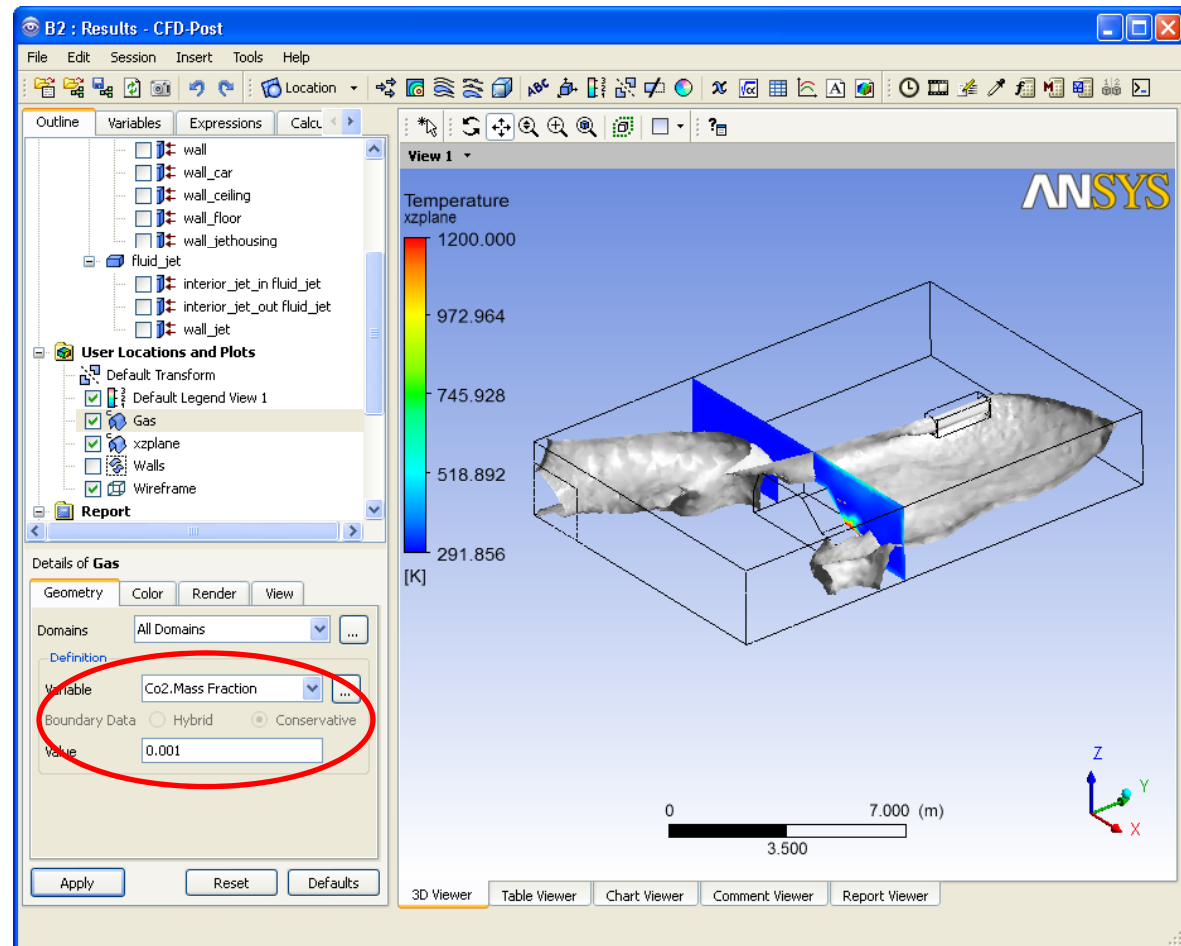
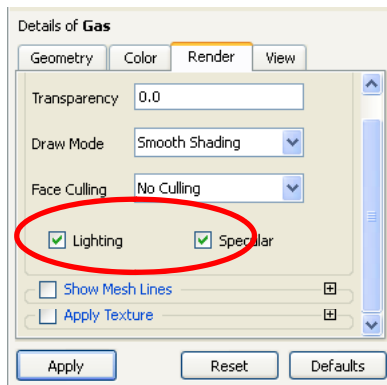
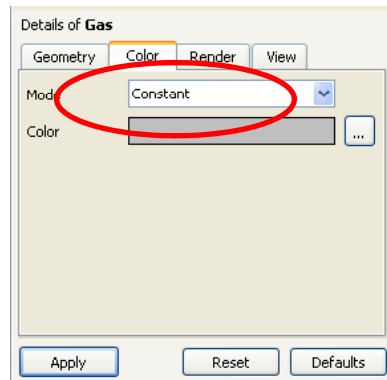
- Define Location details
 - Under Geometry select Y as Variable and set the value to 9 m and set Color and Render as shown below.



- Click Apply. Switch off the previous Location (Walls) by unchecking it in the Outline.

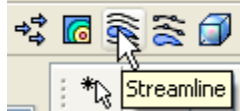


- Add a 3d Isosurface representing gases
 - Use the same procedure - select Locations > Isosurface, enter a name (“Gas”) and click OK.

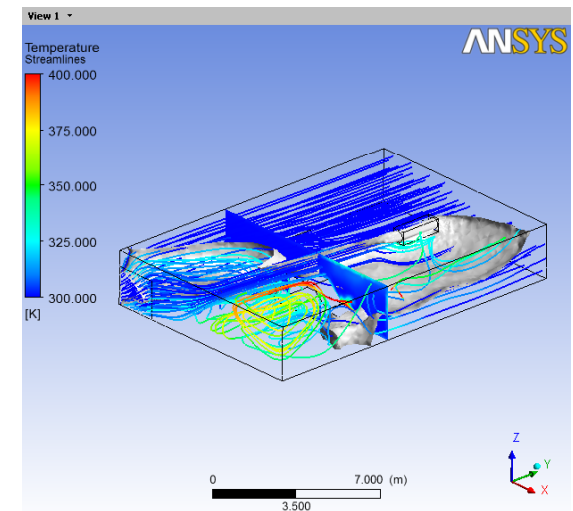
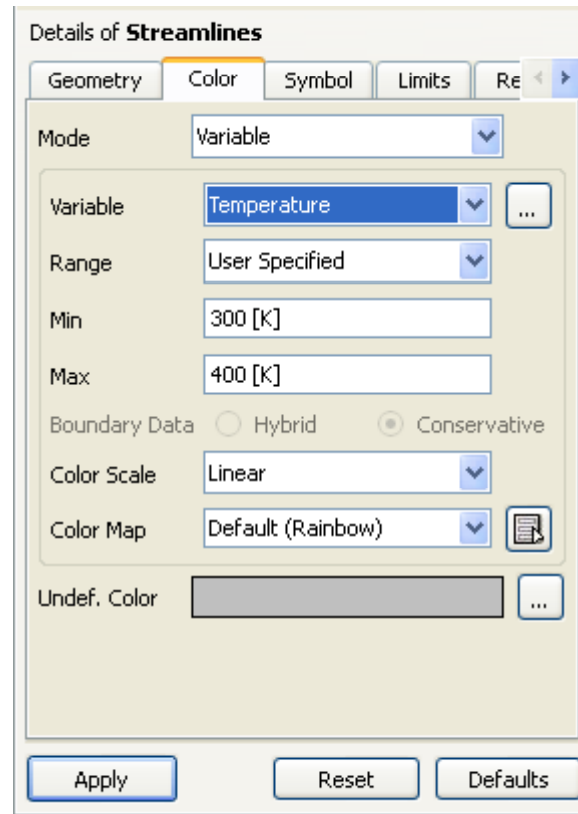
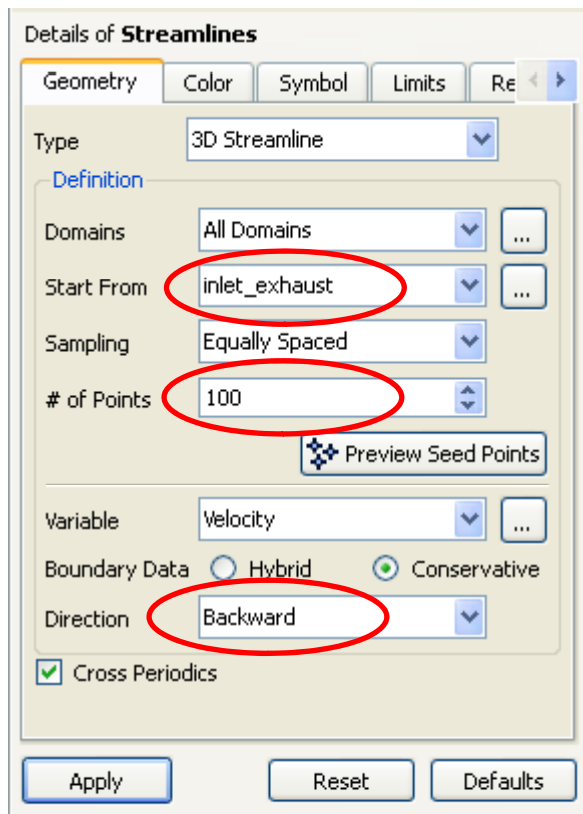


Postprocessing – Streamlines (1)

- Add 3d streamlines to visualize flow

- Click the Streamline button  and enter a name (“Streamlines”).

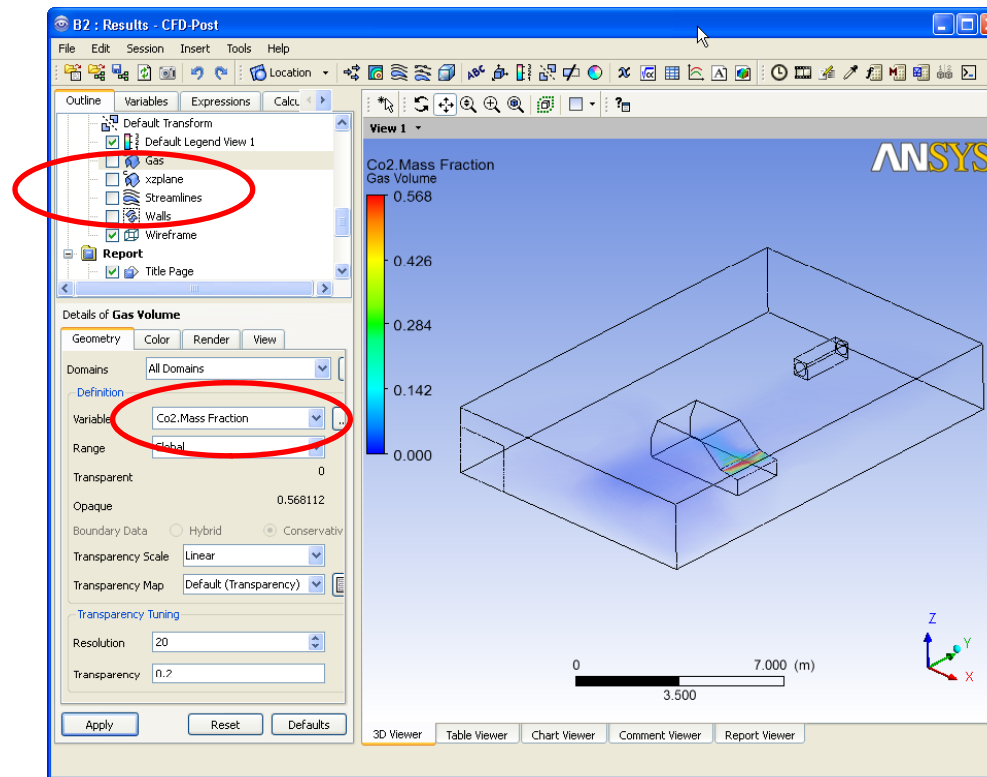
- Apply the Details as shown and click Apply.



Postprocessing – Volume Rendering

- Add Volume Rendering

- Click the Volume Rendering button  and enter a name (“Gas Volume”).
- Apply the settings shown below under the Geometry tab, switch off the other Locations and click Apply.



- Other Features

- There are many other features available in CFD POST
 - Animations
 - Expressions & Functions
 - Charts & Tables
 - Automatic Report Generation
 - Multiple Case Comparison
- Close CFD POST (File > Quit) and save the project from the Workbench Project Page.