

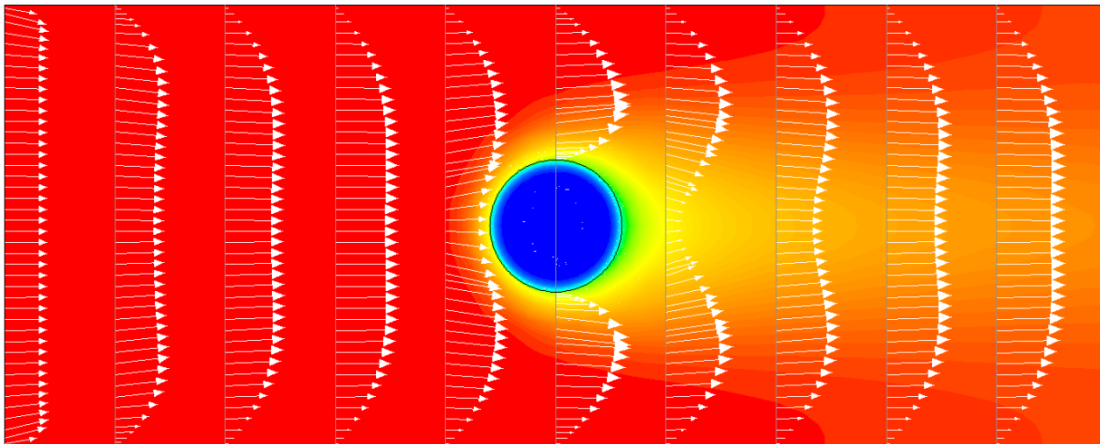
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# Computational Fluid Dynamics for Engineers

## Tutorial 1

### Diffusion and reaction inside a spherical catalyst particle

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This tutorial can be printed and distributed freely in its original and complete form conditioned that it is used as supplementary training material to the book *Computational Fluid Dynamics for Engineers*, Andersson B., Andersson R., Håkansson L., Mortensen M., Sudiyo R., van Wachem B., ISBN 978-1-107-01895-2, published 2011 by Cambridge University Press, The Edinburgh Building, Cambridge CB2 8RU, UK.

Additional resources such as *tutorials, project and lecture notes* are available from the authors and at [www.cambridge.org/9781107018952](http://www.cambridge.org/9781107018952)

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## 1. Tutorial introduction and objectives

The structure of these instructions are as follows.

In Section 1 the problem description is given along with information regarding geometry and boundary conditions. Hence, all information required to solve the problem is found here.

In Section 2 the questions related to the problem, model accuracy and limitations are found, along with instructions on how to prepare a short report.

Section 3-5, contains instructions specific to the Ansys software; how to generate the CAD model, create the mesh, run the simulations and how to do the post-processing. All instructions are written for Ansys Workbench 13 and the software used are: Design Modeler, Meshing Platform, Fluent respectively.

In this tutorial the *flow around and diffusion and reaction inside a spherical catalyst particle* is studied. The purpose is that you, in accordance with best practice guideline, Chapter 7, learn how to:

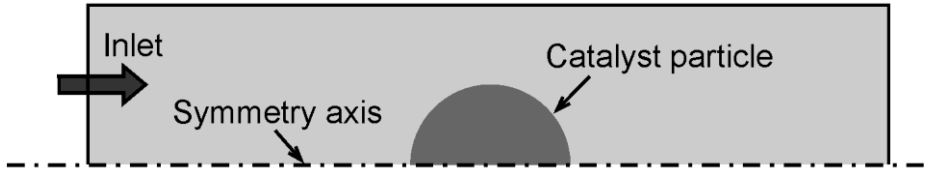
- *Generate* : 2D CAD model and mesh files for the system (2D-axisymmetric model).
- *Analyze*: Mesh quality
- *Define*: Laminar flow with species transport and reaction, transport in porous body.
- *Calculate*: Diffusivity inside porous material, reaction rate, conversion, efficiency factor, mole fractions, species concentration and temperature fields, surface and volume integrals.
- *Judge*: Convergence based on analysis of residuals and species flux at boundaries.
- *Evaluate*: Numerical schemes. Mesh independence.
- *Analyze*: Species composition and conversion at different inlet temperatures. Determine the catalyst effectiveness factor.
- *Discuss*: Validity of simulation results with respect to assumptions made in the problem formulation, limitation with the model, possible refinements.

### 1.1 Tutorial problem description

The purpose of this tutorial is to simulate the reactions that occur within a porous catalyst particle. The system considered in this tutorial is shown in Figure 1.

Ammonia reacts with nitrogen-monoxide to produce nitrogen and water. This process is central in cleaning of exhaust streams from numerous industries, such as power plants. Generally, the reactions are carried out in monolithic reactors, which is the topic of the SCR-project that will be studied later in this course. The reaction rates and diffusivity inside the catalyst are calculated in the CFD-solver using *user*

*defined functions* (UDFs). In this tutorial the UDF, 'tutorial1.c', is appended at the end of this document, it can also be downloaded from [www.cambridge.org/9781107018952](http://www.cambridge.org/9781107018952).



**Figure 1.** Schematic view of the catalyst particle (2D-axisymmetric model).

The following reactions occur in a coated catalyst particle in the centre of the pipe

1.  $S + NH_3 \leftrightarrow S-NH_3$
2.  $S-NH_3 + NO + 1/4 O_2 \rightarrow S + N_2 + 3/2 H_2O$

where S is an active site.

Reaction rate kinetics:

$$r_{1+} = k_{1+} c_{NH_3} (1 - \theta_{NH_3})$$

$$r_{1-} = k_{1-} \theta_{NH_3}$$

$$r_2 = k_2 c_{NO} \theta_{NH_3}$$

Here  $r$  is the reaction rate in molecules per active site and second,  $c$  is the concentration in mole/m<sup>3</sup> and  $\theta_{NH_3}$  is the coverage of  $NH_3$  on the active sites.  $k$  is the rate constant given by the Arrhenius expression.

At steady state the material balance on  $NH_3$  in the porous catalyst ( $S-NH_3$ ) is given by:

$$\left\{ \begin{array}{l} \text{Adsorption} \\ \text{of } NH_3 \end{array} \right\} - \left\{ \begin{array}{l} \text{Desorption} \\ \text{of } NH_3 \end{array} \right\} - \left\{ \begin{array}{l} \text{Consumed } NH_3 \\ \text{by reaction} \end{array} \right\} = 0$$

$$r_{1+} - r_{1-} - r_2 = 0$$

thus giving an expression for the coverage of  $NH_3$ ,

$$\theta_{NH_3} = \frac{k_{1+} \cdot c_{NH_3}}{k_{1-} + k_{1+} \cdot c_{NH_3} + k_2 \cdot c_{NO}}$$

Inserting  $\theta_{NH_3}$  into the rate expression for  $r_2$  gives:

$$r_2 = \frac{k_2 \cdot K \cdot c_{\text{NO}} \cdot c_{\text{NH}_3}}{1 + K \cdot c_{\text{NH}_3} + \frac{k_2}{k_{1-}} \cdot c_{\text{NO}}} \quad [\text{mol/s,site}]$$

Where  $r_2$  is the rate of consumption of ammonia. The reaction rates of the other components are determined from stoichiometry.

The rate constants are given by:

$$k_i = A_i e^{\frac{E_i}{RT}}$$

$$K = \frac{k_{1+}}{k_{1-}}$$

**Table 1.** Kinetic parameters.

Reaction No.	$A_{i+}$ [m <sup>3</sup> /mole,s,site]	$E_{i+}$ [kJ/mole]	$A_{i-}$ [s <sup>-1</sup> ]	$E_{i-}$ [kJ/mole]
1	0.614	0	$1.99 \cdot 10^5$	98
2	$8.39 \cdot 10^5$	59.5	-	-

$A_i$  is the pre-exponential factor and  $E_i$  is the activation energy for reaction i. + denotes forward reaction and - denotes backward reaction.

The reactor is initially operated under the conditions specified in Table 2.

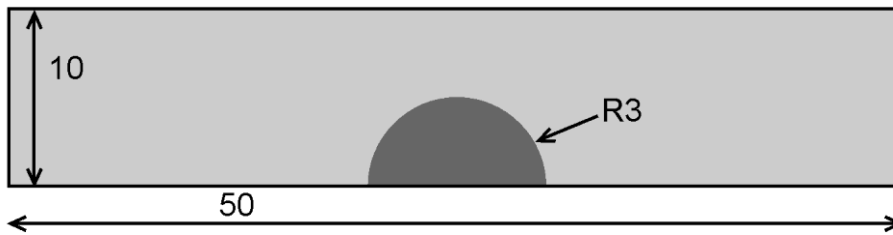
**Table 2.** Boundary conditions.

	Gas inlet	Comment
Velocity	0.1 m/s	
Inlet mole fraction NH3, NO	$5 \cdot 10^{-4}$	
Inlet mole fraction CO2	0.0625	
Inlet mole fraction H2O	0.125	
Inlet mole fraction O2	0.0625	
Inlet mole fraction N2	0.749	
Pressure	101325 Pa	
Inlet temperature	400K	to start with

The porous catalyst is characterized by the following parameters. These are already accounted for in the reaction rate calculations done in the c-file 'tutorial1.C'. You do not need to make any adjustment in this file.

- Effective diffusivity =  $7.68 \cdot 10^{-8} \cdot T^{0.6}$  m<sup>2</sup>/s
- Surface area =  $88 \cdot 10^3$  m<sup>2</sup>/kg
- Active sites per surface area =  $3.48 \cdot 10^{18}$  sites/m<sup>2</sup>
- Density of catalyst = 1770 kg/m<sup>3</sup>
- Sites/m<sup>3</sup> catalyst =  $88 \cdot 10^3 \cdot 1770 \cdot 3.48 \cdot 10^{18} / 6.023 \cdot 10^{23} = 900$  [mol sites/m<sup>3</sup>].

Create your model according to the drawing in Figure 2, and use boundary conditions given in Table 2



**Figure 2.** Drawing of the 2D-axisymmetric model.

**NOTE:** All dimensions are in millimeter.

The spherical catalyst particle is placed in the centre of the pipe, i.e. 25 [mm] downstream from the inlet. The model will later be defined as axi-symmetric. Hence the pipe diameter is 20mm.

## 1.2 Tutorial prerequisites

It is recommended that you have read Chapters 1-3 in the book *Computational Fluid Dynamics for Engineers*. Regardless of what CFD software you use, you will find all required data in Section 1. The questions and tasks related to this tutorial is found in Section 2.

If you use Ansys Workbench you should read Sections 3-5 in this manual to get detailed instructions on how to setup the simulations. If you use any other CFD software you should use the data given in Section 1 to run the simulations and answer the questions in Section 2. Although the menu and structure varies between different CFD software, it is the same input that is needed, and the workflow is very similar: *Geometry->Mesh->Models->Simulation->Post-processing*

## 2. Tasks and report instructions

Turn in a report that focus on analysis of the simulation results and on the following questions:

- Analyze the grid aspect ratio and skewness. Is the mesh quality good? (HINT: Use recommendations for mesh quality in 'Best-practice guidelines' Chapter 7 in the textbook to do this assessment.)
- How is the reaction rate, reaction heat and the effective diffusivity inside the porous catalyst calculated? (HINT for Ansys Fluent users: look into the c-file. You can open the file using a text editor such as Notepad or Wordpad.)
- How does first and second order upwind schemes affect the simulation results ? (HINT Chapter 3.8.3)
- Do you manage to get a grid independent solution, in that case what is required?
- How and why is the effectiveness factor affected by temperature? (HINT see definition below)
- How does the location of the reaction zone depend on the temperature?

*Note: All hints refer to the location in the textbook where you will find an answer.*

### Simulation loop nr 1

Simulate the system according to the specifications in Section 1. (For Ansys Fluent users the three different steps are shown explicitly in Sections 3-5. )

- Make 2D profiles of temperature, velocity and mass fractions.

### Simulation loop nr 2

Change the numerical schemes from first order upwind to higher order and compare the results.

Calculate the catalyst effectiveness factor.

### Simulation loop nr 3

Rerun simulations at 500 and 600 K and compare the results.

### Miscellaneous help

The effectiveness factor is defined as the observed integral reaction rate over the whole particle divided by the reaction rate without influence from mass and heat transfer limitations i.e. the reaction rate with the concentration and temperature outside the pellet.

$$\eta = \frac{\text{reaction rate within the particle}}{\text{reaction rate on the surface of the particle}}$$

$$\eta = \frac{\frac{1}{V} \int r dV}{\frac{2}{A} \int r dA}$$

NOTE: The factor 2 in the denominator should be used in Ansys-Fluent (due to the way reaction rate at the surface is determined)

### Optional exercise

External mass and heat transfer, i.e. the transport outside the pellet, varies at different positions along the periphery. Discuss how the simulated mass and heat fluxes vary from the front to the rear of the pellet. An average of the external mass transfer is usually estimated using the Sherwood number, Sh, which is the ratio of convective to diffusive mass transport.

$$Sh = \frac{k_c d_p}{D} = 2 + 0.6 Re^{1/2} Sc^{1/3} = 2 + 0.6 \left( \frac{u \cdot d_p}{\nu} \right)^{1/2} \left( \frac{\nu}{D} \right)^{1/3}$$

Where u is the mean velocity of the flow around the pellet,  $d_p$  is the diameter of the pellet,  $\nu$  is the kinematic viscosity and D is the molecular diffusivity. The mass transfer is then estimated by (for a sphere):

$$Flux = D \left. \frac{\partial C}{\partial r} \right|_{r=R} = k_c (C_{bulk} - C_{surface}) \quad \text{mol/m}^2\text{s}$$

Calculate the Sherwood number in your simulations at 500 K and compare with the model above. The particle Re number is under these conditions 40. The correlation is derived for a Re number based on a velocity far from the particle or more exact the velocity difference between the bulk velocity and the particle velocity, the particle diameter and the fluid viscosity in the film surrounding the particle. The Sc number ( $\nu/D$ ) is close to 1 in this case with light gases resulting in a Sh number of 5.8

**HINT:** The flux is most easily calculated from the total reaction (molar flow of ammonia into the tube – ammonia flow out of the tube) divided by the outer surface area of the catalyst.

The concentration is calculated from  $C_i = y_i C_{tot} = y_i \frac{P_{tot}}{RT}$  where  $y_i$  is the molar fraction.

NOTE There are several kind of averages:

Surface average  $\bar{C} = \frac{\int C dA}{A}$

Mixed cup average  $C_{mixed\ cup} = \frac{\int v C dA}{\int v dA} = \frac{\int_0^R 2\pi r v(r) C(r) dr}{\int_0^R 2\pi r v(r) dr}$  (for rotational symmetry,  $v(r)$  velocity)

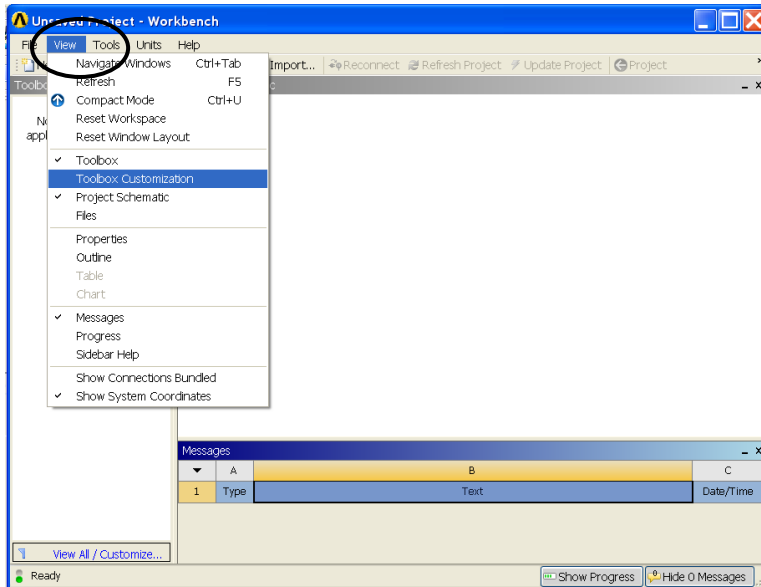


### 3. Instructions for generating the geometry (Ansys 13 Design Modeler)

**Start Workbench** (double-click the Workbench icon on the computer desktop)

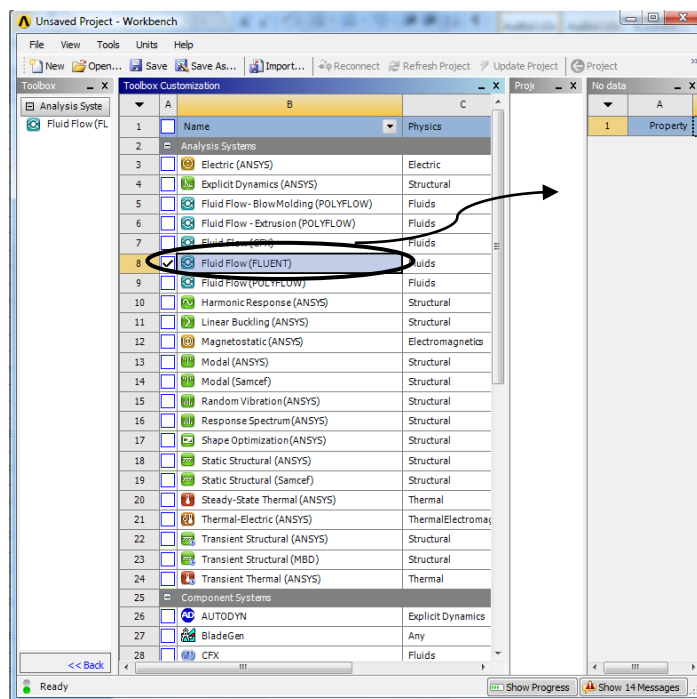
**File: New**

Customize the workbench in **View**



**Mark** Toolbox, Project Schematic and Messages

**View-Toolbox Customization** and select the system you want to use. This allows detailed customizations but at least Fluid Flow (Fluent) must be selected. This customization is enough for this course.

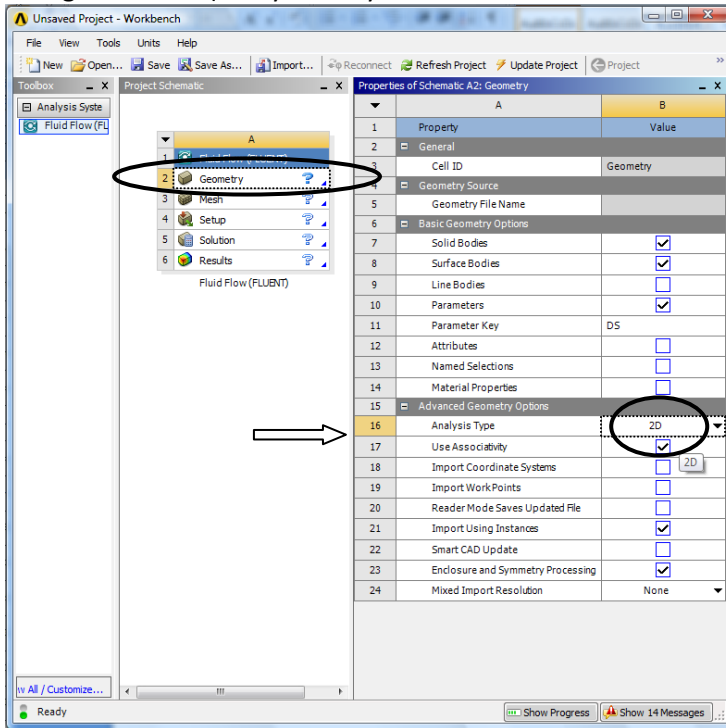


**Drag:** Fluid Flow (FLUENT) into project schematic

Mark **Geometry**

Select: **View –Properties**

Change: **3D→2D** (axi-symmetry is defined later in the CFD solver)

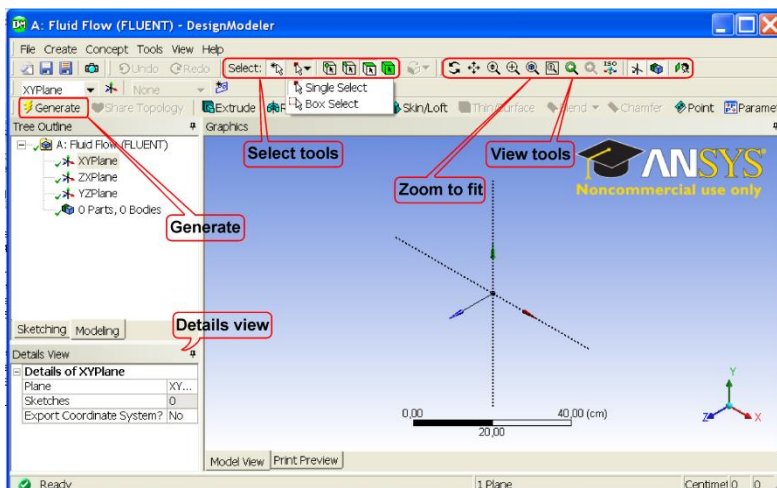


**Double click** on Geometry (or right click and select New Geometry) to start the CAD software. The name of this software is *Design Modeler*

## DesignModeler

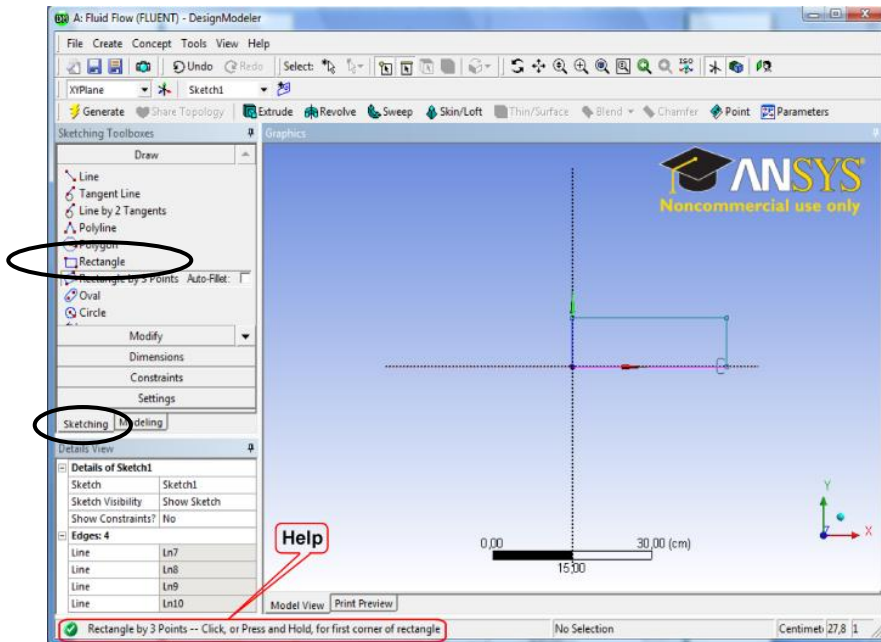
When starting DesignModeler select to work with millimeter or centimeter. In the Figure below you can see the workspace. The most useful icons/tolls are highlighted here for your convenience.

In rotational symmetry, the symmetry axis must be the X-axis to avoid conflicts inside the CFD-solver (Fluent). You can select the XYPlane or ZXPlane for that purpose. Here we have chosen the XYPlane.



Select the view angle by clicking on 'z' on the coordinate-system-icon in the lower right corner (or right click the mouse within the drawing screen and **View**-e.g. Front View)

There are two basic modes in this program: *sketching and modeling*. We start with sketching to generate the sketch and put constraints and dimensions to the drawing.



**Select:** Sketching-Draw-Rectangle (the exact dimensions of the rectangle is not important at this stage, you will later specify its exact shape)

First we draw the pipe in 2D rotational symmetry. Draw a rectangle (you will adjust the size later). A letter C indicates that the line is snapped onto the axis and P indicates origo.

NOTE Since you use the X-axis as symmetry axis you are not allowed to draw below the X-axis (negative Y).

You can anytime undo the last step in your drawing by clicking **undo**.

**Select:** Dimension

Click on the line and drag it to the side. (Do not drag too far or the dimension lines will be far from the body)

Set the dimensions: Length 50 mm and height 10 mm

To do this the box in the details view has to be unmarked. If you mark the box in details view, you have the opportunity to name the parameters and later change the dimensions by altering the parameters. (We will not use that in this tutorial, but you may use it in the project late on in the course).

Press **Generate** when you are satisfied. You can zoom the windows to fit.

Go to **Modeling** by selecting the modeling tab as shown in the Figure below. This is the second mode of the program and is used when the sketches are done.

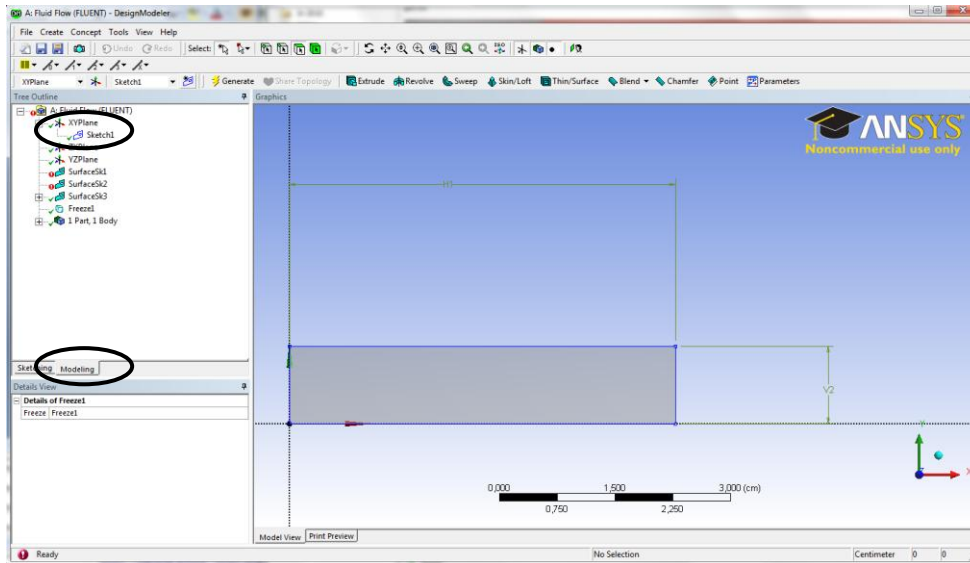
Select and expand XYPlane and select Sketch 1

**Concept-Surfaces from Sketches** to obtain a surface. **Generate**

Use **Freeze** under **Tools** to keep the geometry intact. If you do not freeze the geometry it will blend into other parts of the geometry i.e. the catalyst.

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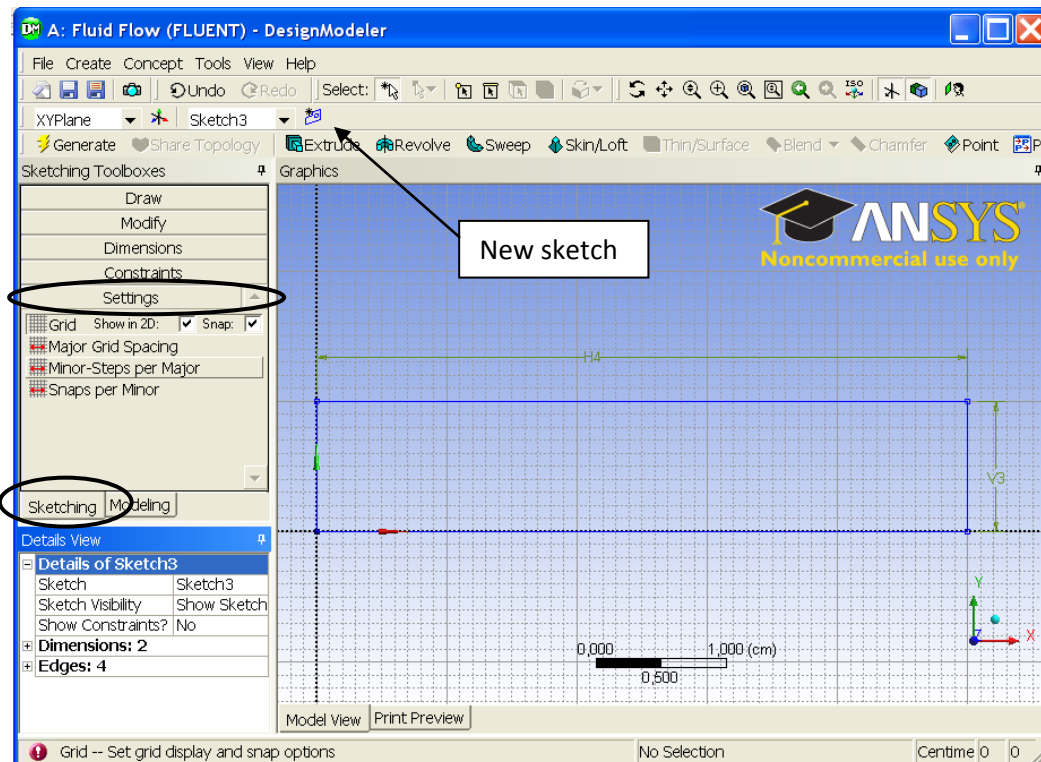
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Now we will add the catalyst particle. Go back to the **sketching** mode.

We can use a grid to help putting the catalyst on the right place (25mm from the inlet).

Select **sketching** mode: **Settings** and choose grid 2D and snap. **Major grid** 10 mm. **Minor-Steps** 10 and **Snaps per Minor** 1.

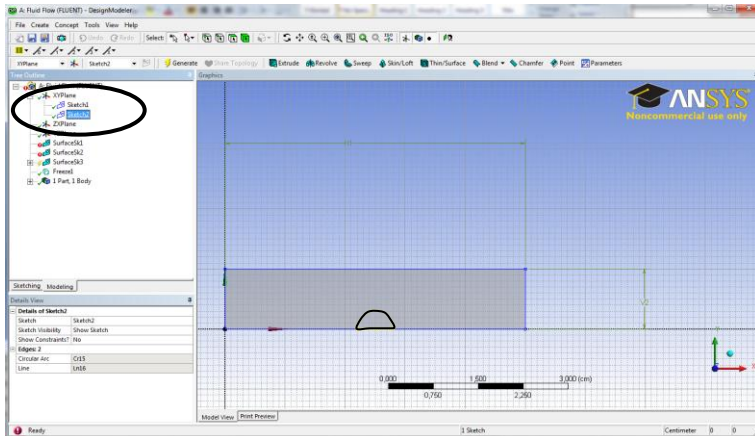


We must draw the catalyst in the same plane (XY) but in an new sketch.  
Therefore press **New Sketch** and mark Sketch2

Select **Draw** and draw an **arc by center** on the X-axis 25 mm from the edge.  
Select the Dimensions and specify the radius 3 mm.

Draw a straight line to form a closed half circle. (P will mark that you have selected the edge of the half circle.

Go to **Modeling** and mark Sketch2 and press **Generate**



With Sketch2 marked go to **Concept-Surfaces from Sketches** to define a new surface. **Generate**  
Go to **Tools** and press **Freeze**.

At this point two surfaces exists that are overlapping each other The next step is to separate the catalyst from the pipe. This is done using a Boolean operation, where the half circle (tool body) is subtracted from the rectangle (target body), mean while preserving the tool body.

### Create - Boolean Operation - Subtract

Expand 2 Parts 2 Bodies

#### Target Bodies

Mark the surface that corresponds to the rectangle from the expanded list 2 Parts 2 Bodies

**Apply**

#### Tool Bodies

Select the half circle from the list

**Apply**

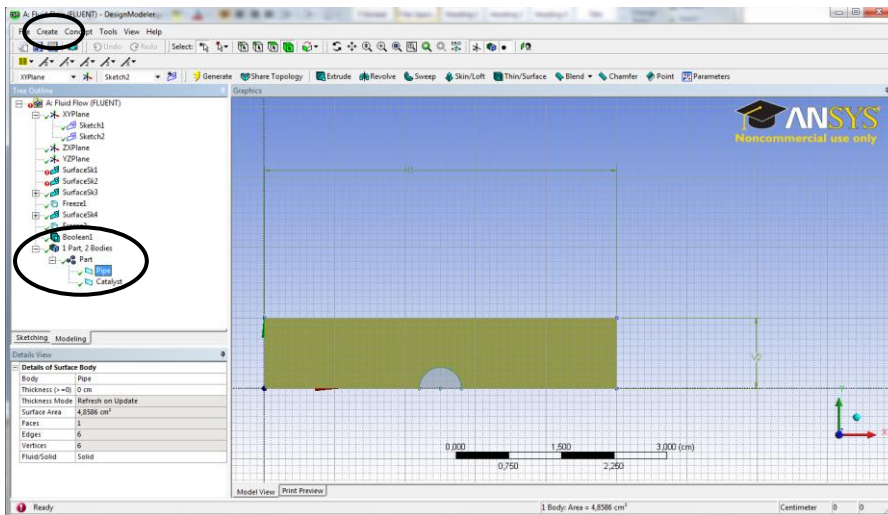
#### Preserve Tool Bodies?

Yes

(This is necessary or only a hole will remain where the catalyst is located)

#### Generate

(If you click on 2 Parts 2 Bodies you will see that the bodies are separated.)



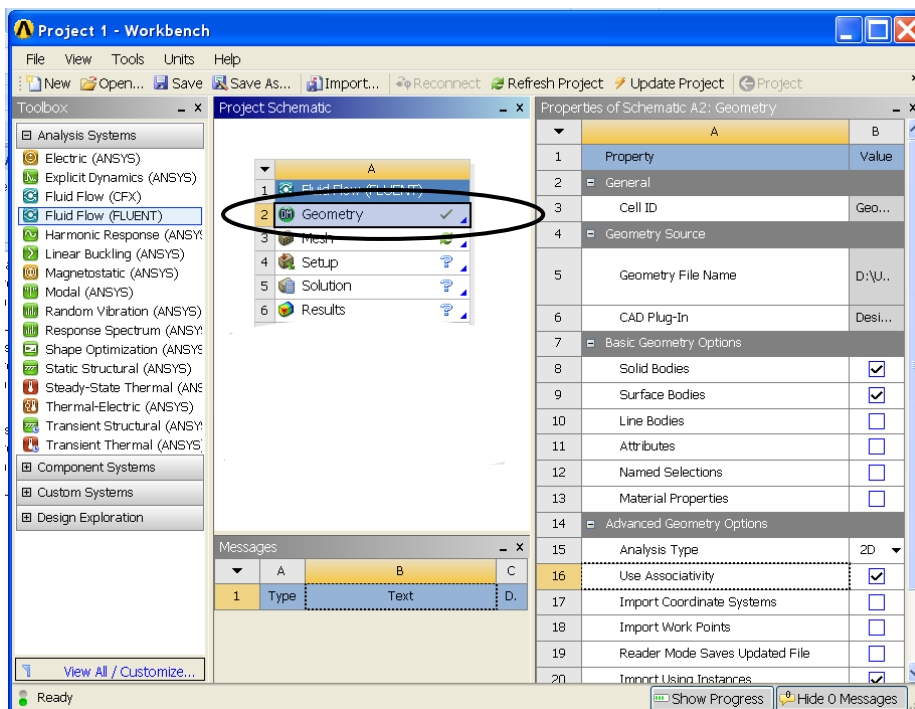
You should now rename your bodies (e.g. Tube and Catalyst) by right clicking on the names in the expanded list.


In order to Mesh the bodies together they must form one Part (multibody part). Therefore mark the two bodies in the list and right click and select **Form New Part**. (You can also name this new part)

**Generate**

**Save Project.**

Back in the Workbench it should look like this



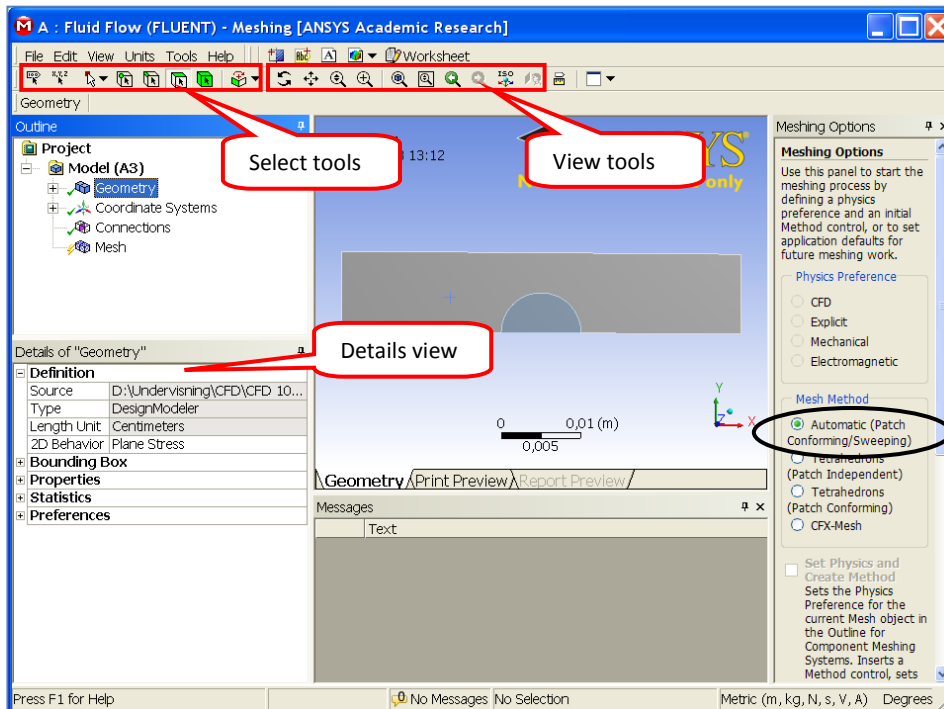
NOTE: Geometry is updated. It is marked OK,  in green.

If you have any other mark you have to go back to Geometry and correct your drawing. The most common error is that you forgot to press Generate.



## 4. Instructions for generating the computational mesh (Ansys 13 Meshing Platform)

In Workbench - Right click **Mesh** and Edit (or double click). This will start the meshing program. The most useful tools are highlighted for your convenience in the Figure below.



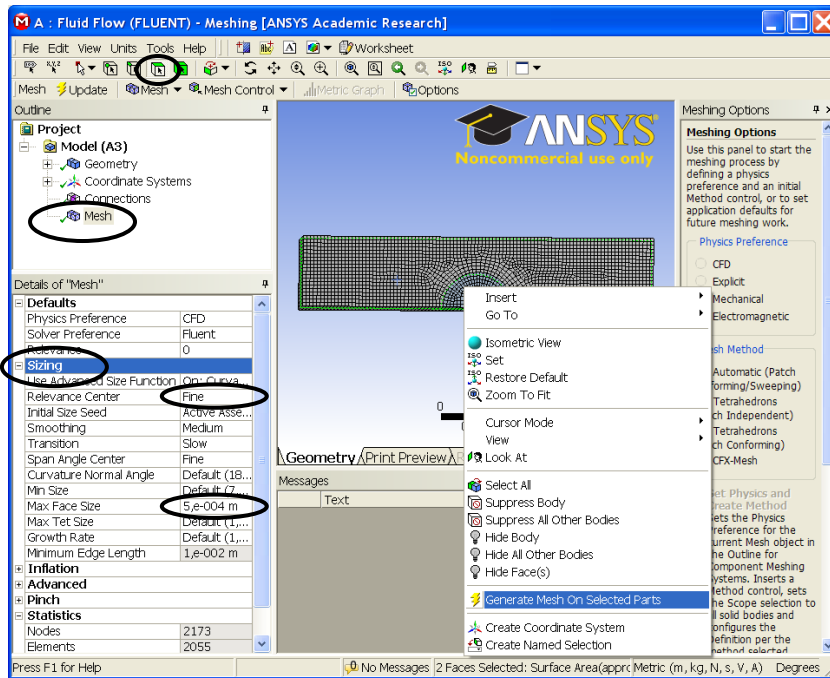
In order to generate your first mesh you first select Mesh in the project outline tree.

Mesh control -retain the default setting - automatic (this option is located on the right hand side in the figure).

Select the surface to mesh (either use Box Select or ctrl Left Click on **all** parts of the body).

Select **Mesh** and change Relevance Center to Fine and Max Face Size to 5.0 e-1 mm in **Details of Mesh-Sizing** as shown in the Figure below.

**Mesh** right click on the surfaces you want to mesh i.e. all surfaces and **Generate Mesh on Selected Parts**



The next step is to specify names for all the parts in the system that we later need to identify in Fluent when we should specify boundary conditions.

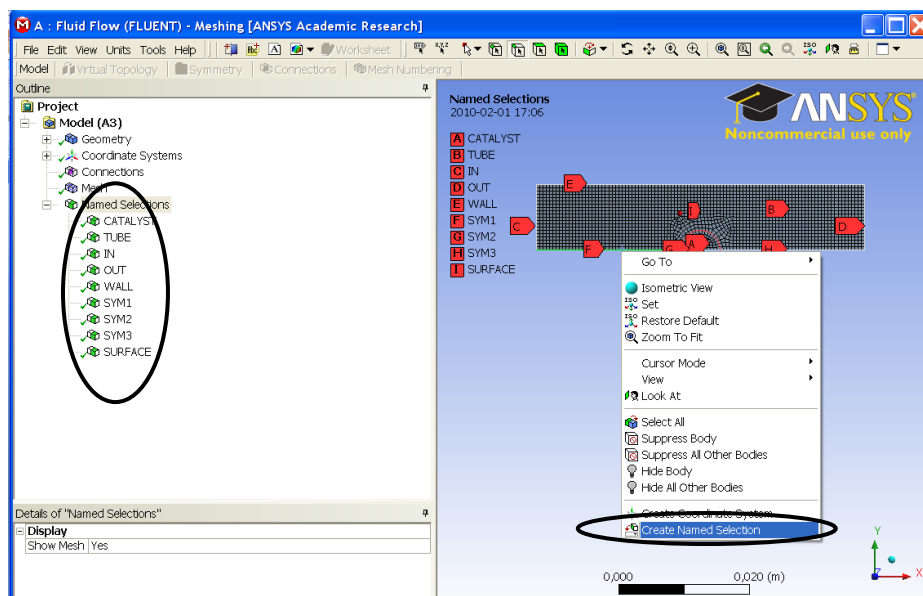
Select the icon **Face** in the top row as show above in the Figure.

First select one of the two surfaces by left-clicking and then right click on the selected surface and **Create Named Selection** (Catalyst or Tube), as shown in the Figure below. Do this for both surfaces.

Select the icon **Edge** (located to the left hand side of Face in the top row) and give names to all the edges: IN, OUT, Sym1 Sym2, Sym3 and Wall (or whatever name you like).

Specify the name of the Catalyst and Tube interface e.g. Surface.


HINT if you select the names Axis1-3 and Vin, Fluent will recognize them as axis and inlet velocity. You will later specify boundary conditions for these edges in Fluent.





Select **Mesh** again and **Update**.

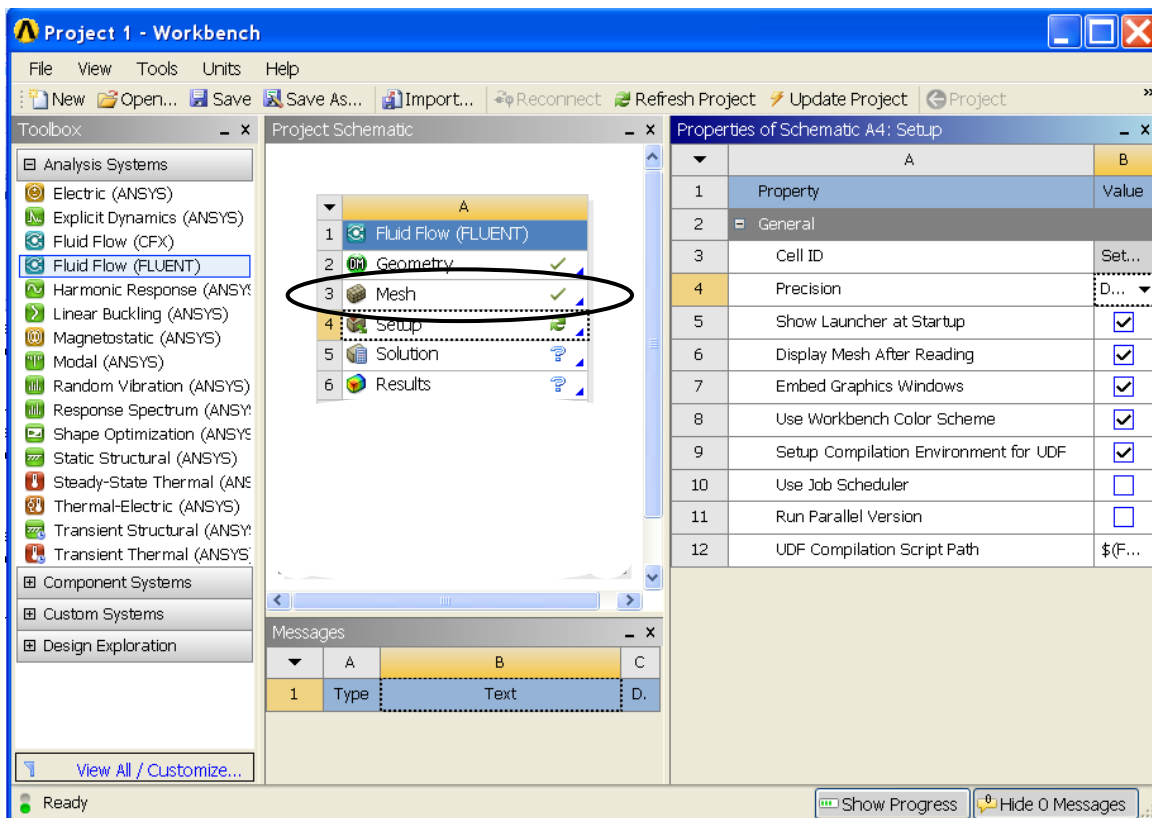
**Save.**

Go back to Workbench. The Mesh is now updated, it is marked OK,  in green. If you have any other mark you have to go back to the Meshing program and correct your mesh. If you do not get OK you probably forgot to press update in the Meshing program.

**Save** the project.

Preferably you also make a copy of the project after meshing is completed. **Save as** (new name).

This allows quick recovery of the model in the case the computer crashes, or if you make a sever mistake in setting up the model.





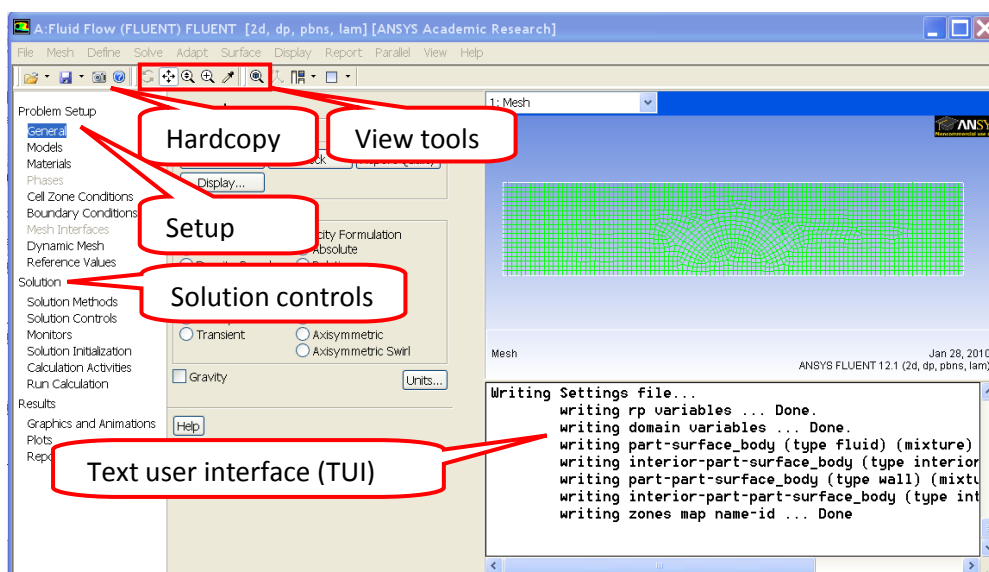
## 5. Instructions for running the simulations (Ansys 13 Fluent)

Begin with downloading tutorial1.C to your user directory, [www.cambridge.org/9781107018952](http://www.cambridge.org/9781107018952).

tutorial1.C is a C-program that calculates reaction rates, heat of reaction and the effective diffusivity in the catalyst particle in Tutorial 1.

In Workbench - Right click **Setup** and select Edit to start Fluent. Start Fluent in double precision.

The most useful tools are highlighted for your convenience in the Figure below.



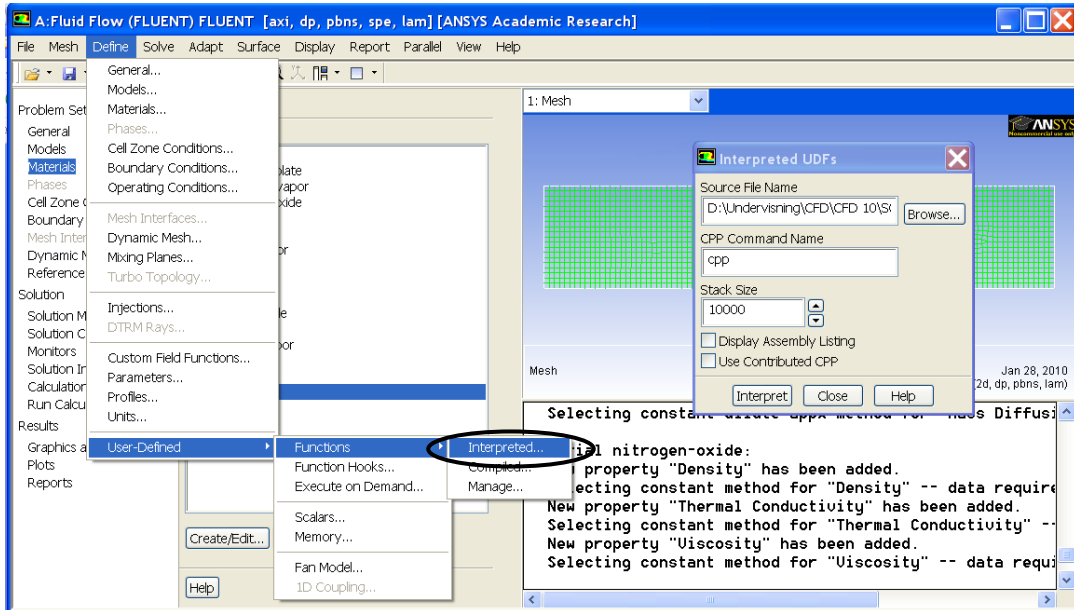
In Fluent the work flow is straightforward. You start from the top left: *Problem setup*, then you apply *Solutions controls* and run calculations. You have access to various tools under *Results* that help to interpret and analyze the results e.g. surface and volume integrals, calculate fluxes. These particular tools are used in Tutorial 1. There is a large selection of visualization tools, you can easily make contour and vector plots for example.

First we need to read the user defined functions (tutorial1.c) that calculates the reaction rates etc into Fluent.

(If you are interested how this file looks like you can open and read it using Notepad)

**Define – User – Defined – Functions - Interpreted** and select tutorial1.C and **Interpret** (as shown in the Figure below)

You must also set **Define – User – Defined –Memory -user defined memory =1**. The reaction rate will be stored in that memory.



### Problem Setup - General

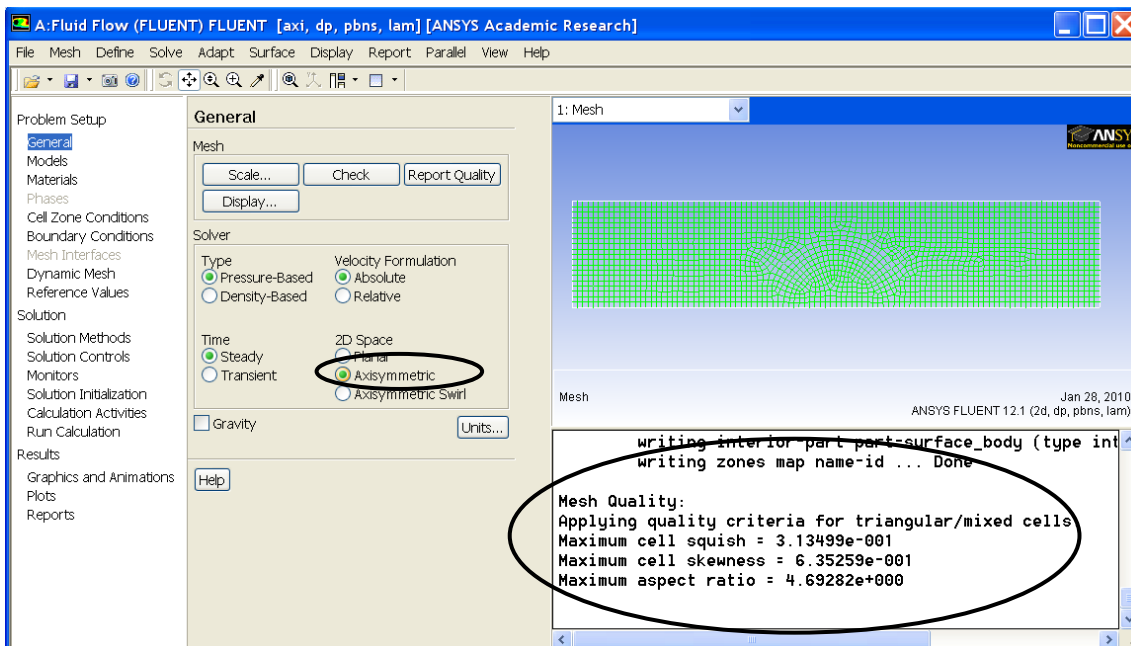
You can make a quick assessment of the mesh quality, inside Fluent if you have not done that in the meshing program.

Report Quality Check **Mesh-Info-Quality**.

Note that the results are printed in the text user interface (lower right corner/promt). These numbers can be compared to the recommended limits given in *Chapter 7 Best Practice Guidelines*, in the text book.

The next step is to specify a axisymmetric model.

Select **General - Solver – Axisymmetric**



You can use the middle mouse button and move around the mesh to make it fit the window.

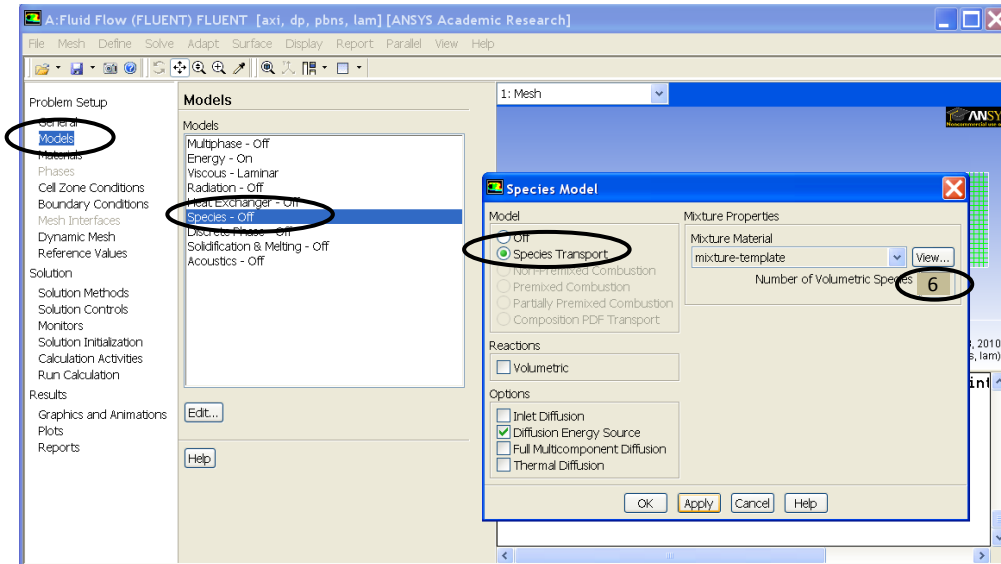
You can also use the zoom function to fit the mesh to the screen.

## Models

Under model you select **Energy on** since you will calculate reaction heat and the temperature.

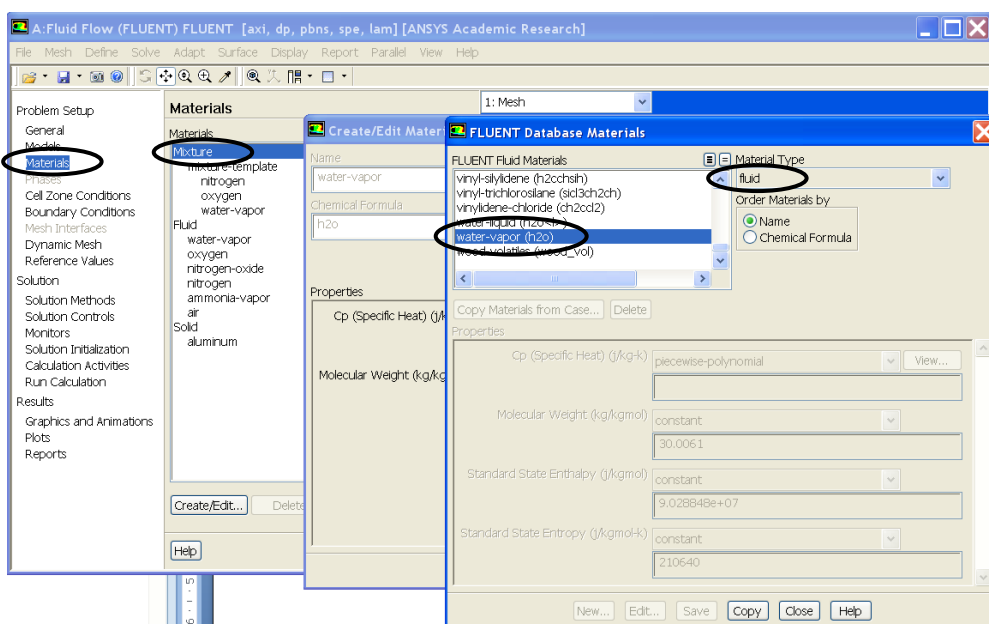
The flow is **Laminar (Viscous - Laminar)** retain the default setting.

**Species Model (Species - Species transport)** and enable 6 number of species, as shown in the Figure below.

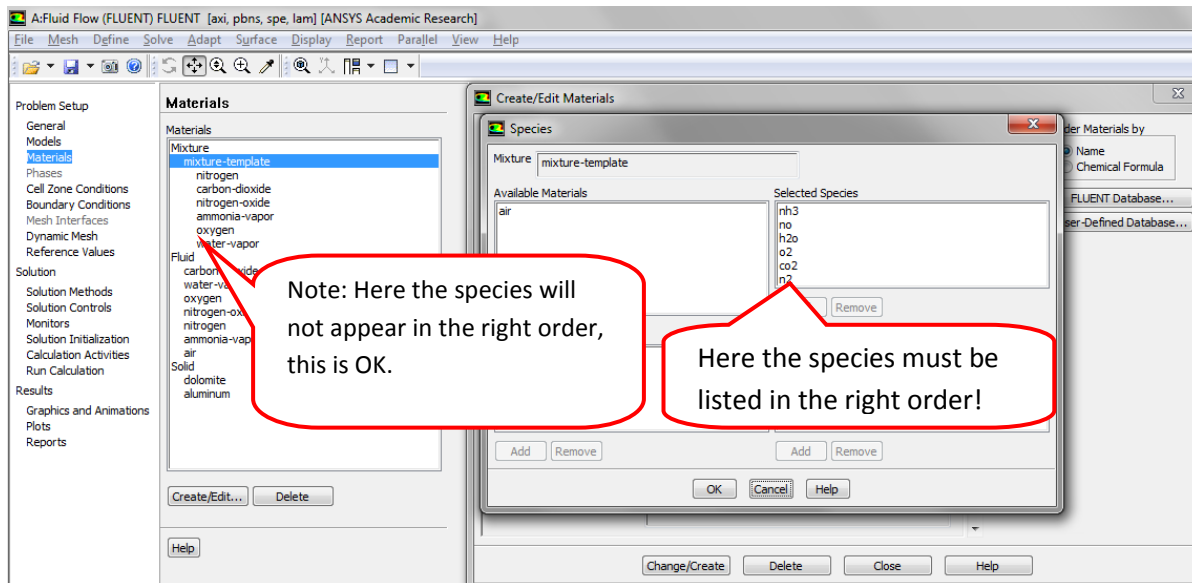


It is possible to use a built in chemical reactions panel. But will in this tutorial we use the **User Defined Function (UDF)** to calculate the reaction rates and diffusivities in the catalyst. However, first we must define all our components in the Mixture Template.

**Material>Create/Edit – FLUENT DATABASE** Select **Fluid** and mark ammonia-vapor, nitrogen, nitrogen oxide, oxygen, carbon dioxide and water vapor and then push Copy. Also select a solid compound that has similar properties as your catalyst e.g. dolomite and then push Copy. Once you have made a selection you can change the properties (and the name if appropriate).



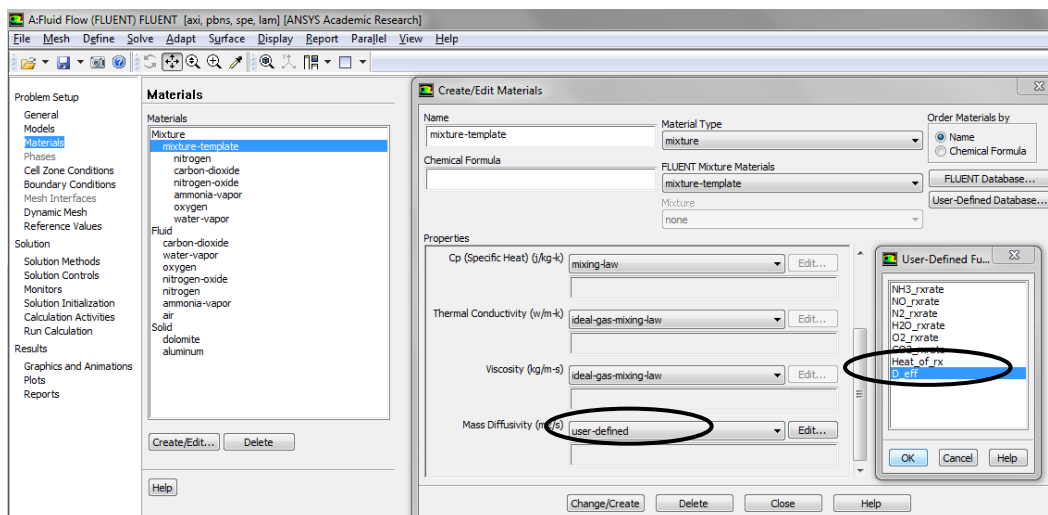
In **Materials-Mixture templates-Mixture Species** select the species in the given order nh3, no, h2o, o2 co2 and put n2 last. The largest component should be last since the last component is not calculated from transport equations but determined from the total balance. (Since we do not need air, it can be removed in the **Materials Menu**)



The properties of the **Mixture** is defined in Mixture **mixture-template**. Set density to incompressible-ideal-gas, Cp to Mixing Law and thermal conductivity and viscosity to ideal-gas mixing law. For mass diffusivity enable 'user-defined' and use UDF 'D\_eff', as shown in the Figure below.

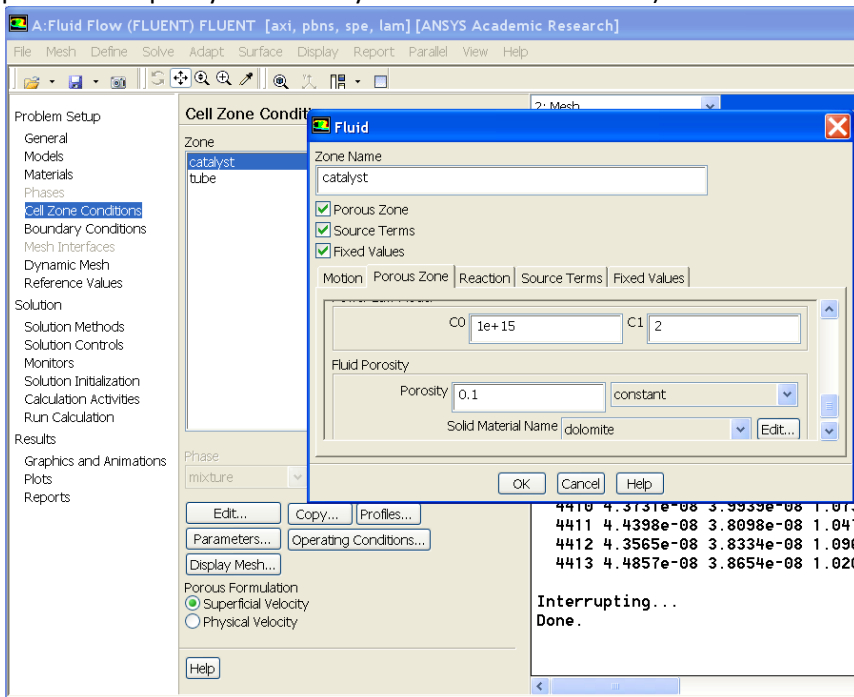
Press Change/Create and close the panel.

Change the viscosity and Cp for all the individual components to Kinetic Theory. This will introduce a temperature and pressure dependence on these properties. The default values are constant values. NOTE It is the **mixture template** compounds that you should change not the fluid components.



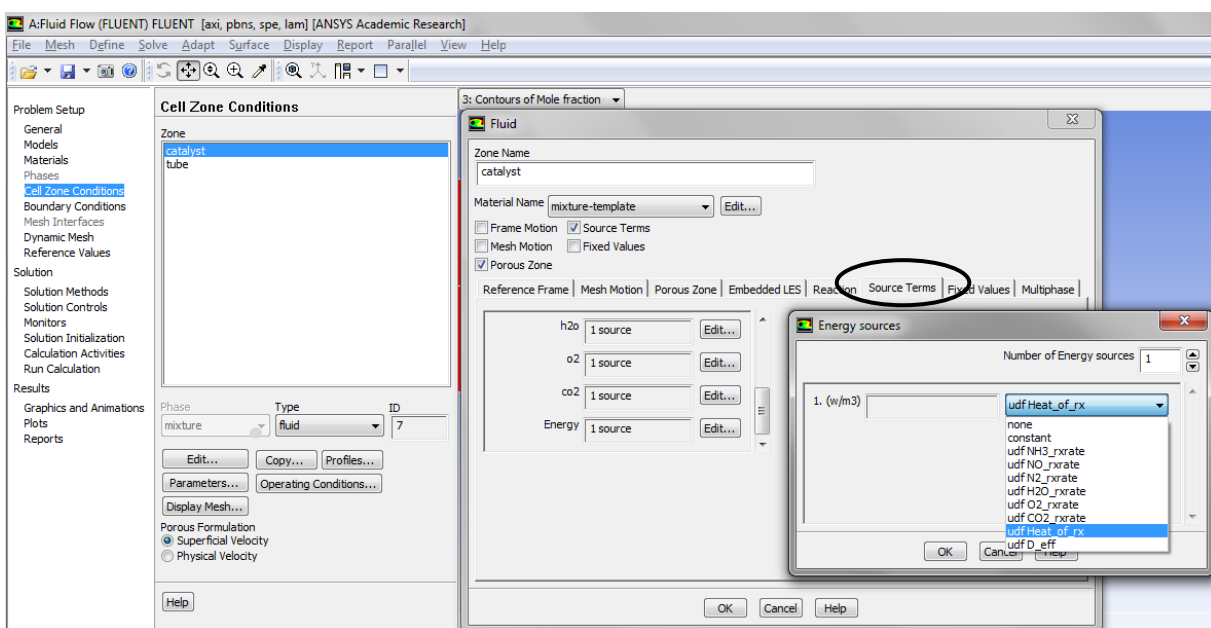
Select **Cell Zone Conditions** – catalyst - Edit - **Porous Zone** and set  $C_0=1e15$ ,  $C_1=2$  and porosity =0.1, shown in the Figure below.

Using the Power Law model the pressure drop is calculated from  $\frac{\partial P}{\partial x_i} = C_0|v|^{C_1-1}v_i$ . This flow resistance will hinder convective flow through the porous catalyst and the only transport mechanism will be species diffusion and heat conduction. (Since the velocity is very low inside the porous zone, it would have been possible to specify the velocity as zero in **Fixed Values**.)



Set the **Solid Material** to Dolomite (the last line in Porous Zone, you might need to scroll down to find it)

Select **Source Terms** and **Edit** the source terms for all Species and the Energy, as shown below. These source terms are fetched from the UDF file.



For the Cell Zone **tube** you only choose Type **fluid**.

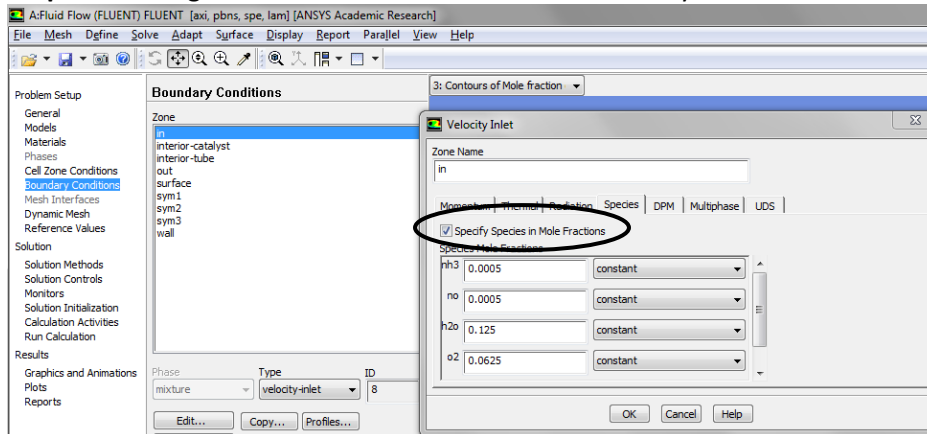
In Boundary Conditions we set the conditions on all boundaries starting with inlet.

Choose **velocity-inlet** for **Type** and then **Edit**.

In **Momentum** set the velocity specification method to 'normal to boundary' and specify the velocity magnitude 0.1 m/s.

In **Thermal** set inlet temperature to 400K. The conversion will be very low at this temperature, but conversion is easily obtained. Later in the tutorial you will increase the temperature. This increase may cause convergence problems and the under relaxation for energy (and maybe species) must be decreased.

In **Species** change to *Mole Fractions* and set the boundary conditions according to **Table 2**.



Set Interior-catalyst, Interior-tube and Surface as **Interior** to allow transport through these regions.

Change Sym1, Sym2, and Sym3 zone type to **Axis**.

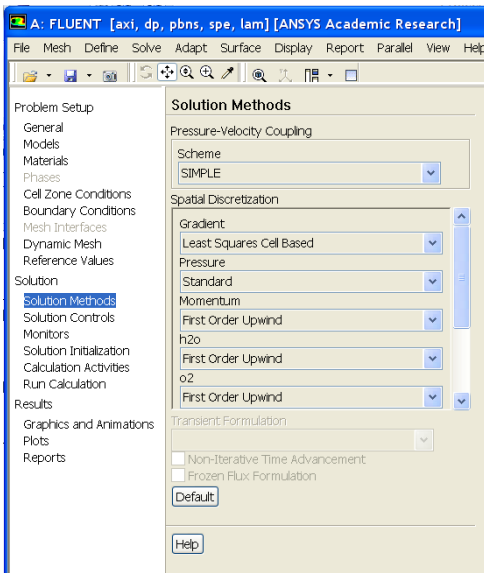
**Change** Out zone type to **Outflow** and Wall zone type to **Wall**.

Set **Boundary Conditions – Operation Conditions- Operating Pressure** to 1 atm (retain the default operating pressure 101325 Pa).

## Solution

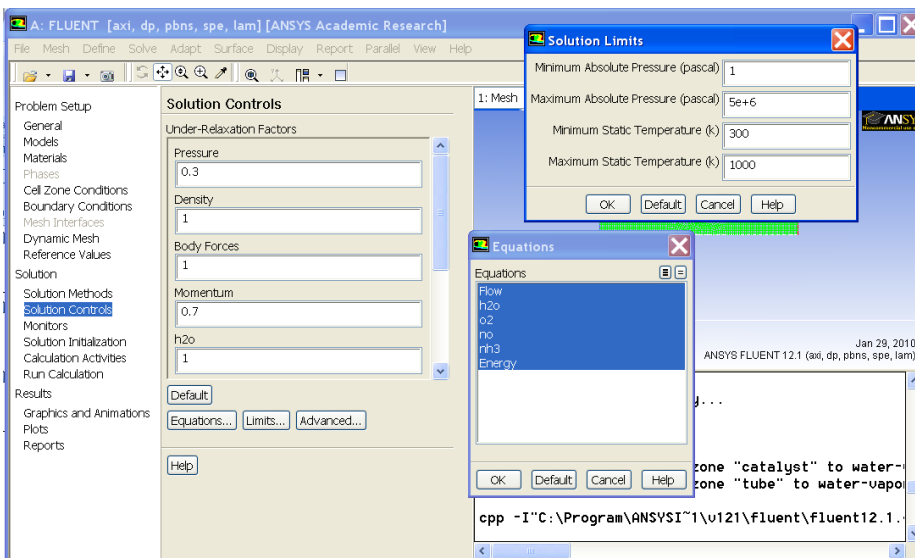
In the solution methods panel we can keep the default settings at the moment. The First Order Upwind schemes are very robust and are recommended for the initial iterations. However, these methods may introduce large numerical diffusion and you should always change to a higher order method at the end of the iterations and compare the solutions. You find more information on these schemes in Chapter 3 in the textbook.



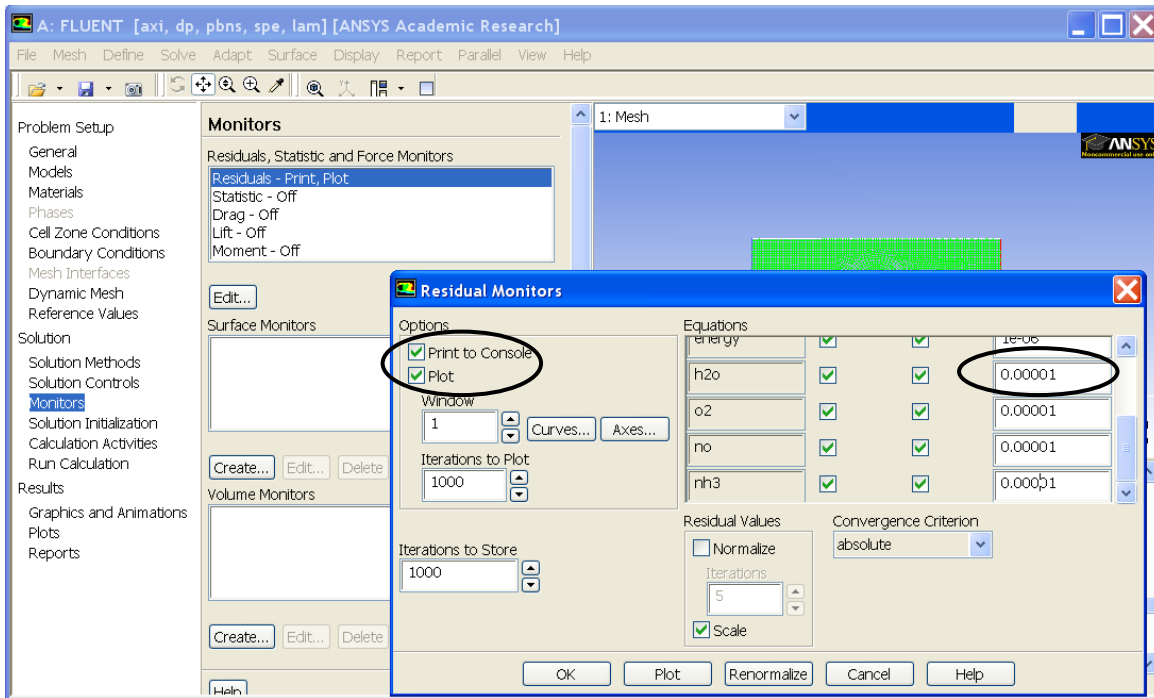


In Solution Control you can use the default values. You also have the opportunity to specify what equations that should be solved. We should keep all equations at the moment but if we have low concentrations and small heat effects we might solve Flow first and then Species and Energy separately. If you have convergence problems it may be a good practice to solve one equation at the time.

Solution limits can also be modified. If Fluent during the iterations reaches extreme values, it can be easier for the program to find its way back. Select limits that are clearly outside your expected range.

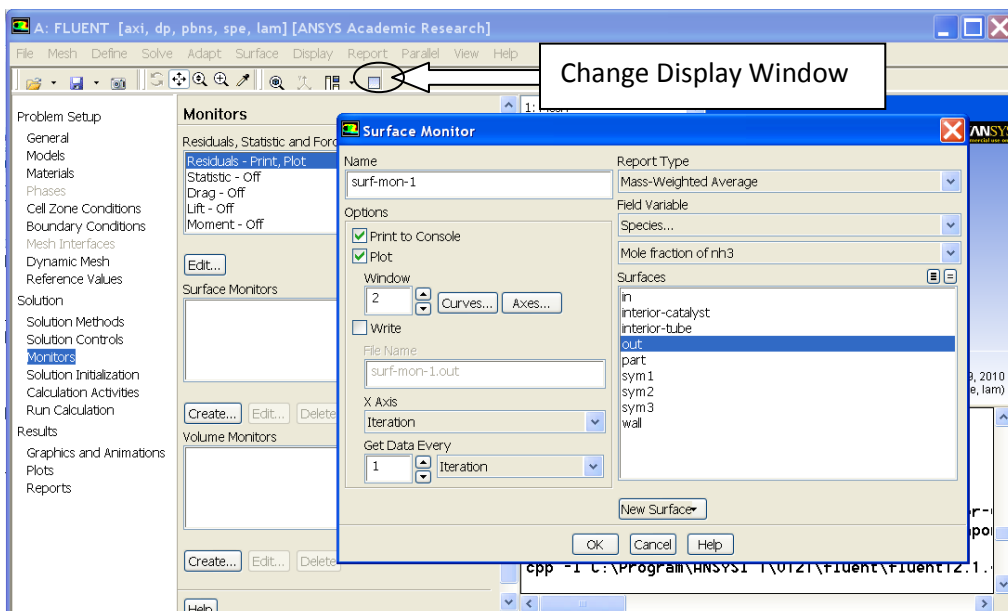


In Monitors you select how to follow the iterations to convergence. Select Print to Console and Plot. You must also change the Convergence limits for the species to  $1 \cdot 10^{-7}$ . If the outlet concentration has not reached a steady value the convergence limits must be decreased further.

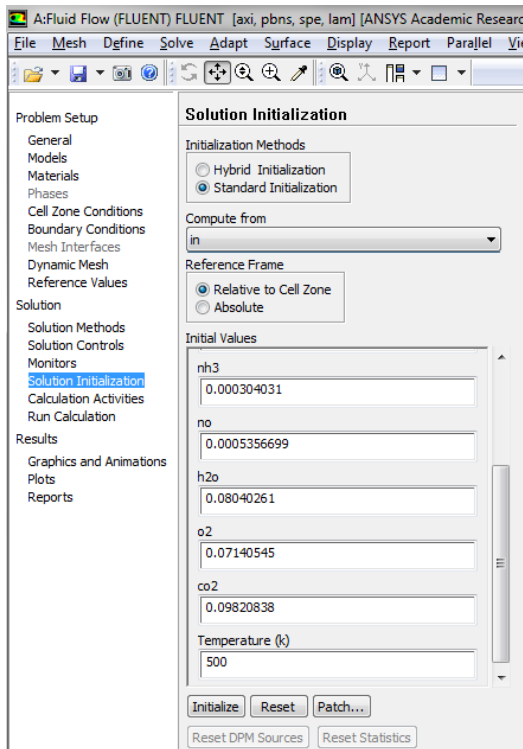


It might be difficult to estimate when convergence is reached from the residuals. A usefully method to follow the iterations towards convergence is to monitor certain variables. In this case to monitor the average reactant concentration in the outflow.

Select Create in **Surface Monitors**. You should also specify in what window you want the plot to appear. Also split the display widow so both the residual and the average concentration can be shown at the same time (use the icon "arrange the graphics window layout").



You must specify initial conditions before starting the iterations. The better you can specify the initial conditions the easier to find the solution. In this case we initialize by **Compute from** select the inlet conditions. Press **Initialize**.



In **Calculation Activities** you can select Autosave this is often very important, but not in this tutorial since the calculations are very fast.

**Save Project** (you can save it under a new name as a backup)

To run the calculation, specify 1000 iterations under **Run Calculation** and press **Calculate**.

When you have obtained a solution go to graphics and animations **Contours-Setup** to study the solution. Here you can make contour and vector plots.

Save pictures of temperature and some species by clicking the camera (icon) in the toolbar.

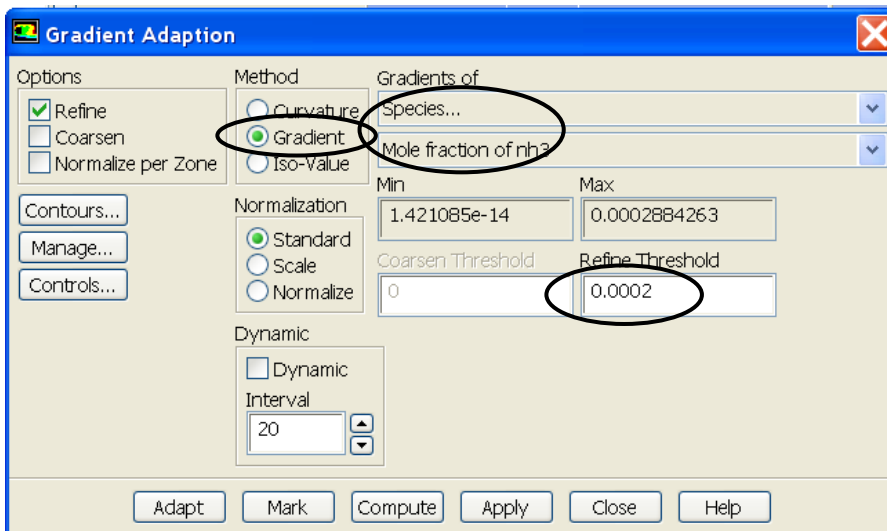
In this first simulation loop we have used a very coarse grid in order to minimize computational time. An efficient way to improve the mesh is to adapt the mesh in areas where most changes occur, i.e. regions with large gradients.

#### Refining the Mesh

**Adapt-Gradient** and select **Gradient** and mole fraction of NH3. **Compute** to obtain an estimation of existing gradients and define a threshold, **Refine Threshold**, select a suitable number (lower than the maximum), as shown in the Figure below.

In this simulation you should specify the **Refine Threshold** so the number of cells in the mesh increase approximately 100-200 cells (the value 0.0002 below may be too high).

Click **Mark** to see how many cells that will be added (given the specified threshold value, if needed adjust it). Finally click **Adapt** to make the change (NOTE: only press Adapt once).



To view the new Mesh **Display -Mesh**

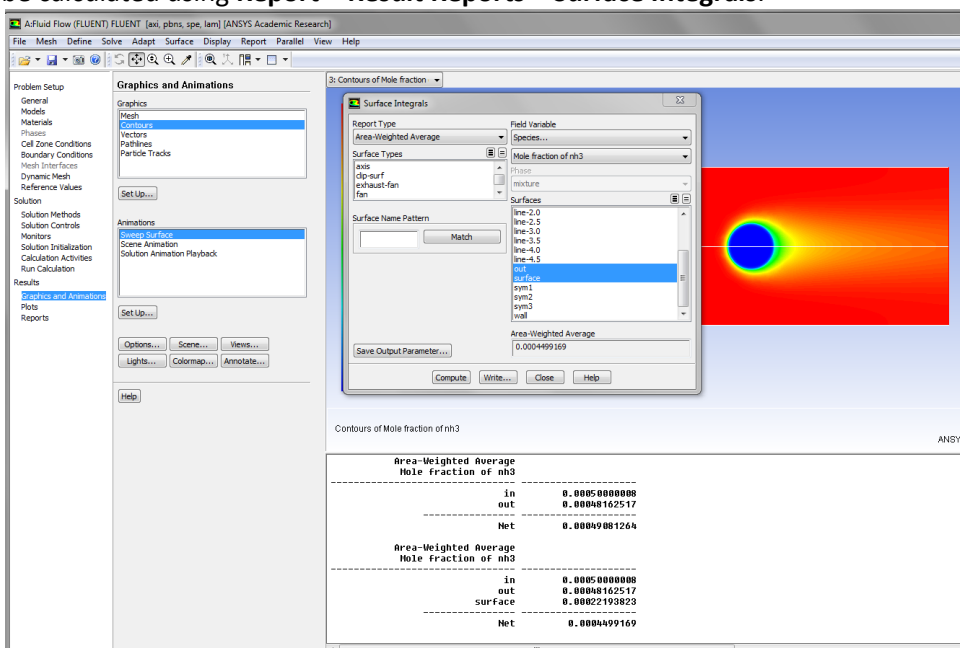
Rerun the simulation without initialization. Instead we use the existing solution (from the coarse mesh) as starting point for the refined mesh. **Solve** and run the simulation until convergence.

In Solve-Method change the numerical schemes to *higher order* in order to decrease numerical diffusion. Rerun the simulations once again.

**Solve** and compare the results with the previous results using first order upwind.

## Post -processing

HINT: The effectiveness factor can be estimated from the net difference between inflow and outflow of e.g. NH<sub>3</sub> compared to the reaction rate using the surface concentrations. The surface concentrations can be calculated using **Report – Result Reports – Surface Integrals**.



HINT: The Sherwood number is calculated from the bulk concentration (Inlet), surface concentration and the net flux (moles/m<sup>2</sup> catalyst surface).

**C-program** tutorial1.C (Windows version, comments and CR (Carriage Return) are different in Linux)

```
#include <udf.h>

//      Constants
real Av=6.22e23;           //      [molecules/mole]
real NAS=3.48e18;          //      [sites/m2]
real Sa=88.e3;             //      [m2/kg]
real ro=1770.;             //      [kg/m3]
real R=8.314;              //      [J/K/mol]
real M_NO=0.0300061;       //      [kg/mol]
real M_NH3=0.01703061;     //      [kg/mol]
real M_N2=0.0280134;       //      [kg/mol]
real M_H2O=0.0180154;      //      [kg/mol]
real M_O2=0.0319988;       //      [kg/mol]
real M_CO2=0.04400995;     //      [kg/mol]
real dH=407000.;           //      [J/mol]

//      Operating pressure
real Pinn=101325.;

//      Variables
real T,P,Ctot,y_NO,y_NH3;  // Temperature, pressure, total
                             // concentration, mass fractions
real k[3],E[3],A[3],K;     // Parameters

enum{nh3,no,h2o,o2,co2,n2};

DEFINE_SOURCE(NH3_rxrate,c,t,dS,eqn)
{
    real den,CNO,CNH3,Ptot,source;
    int i;
    den=C_R(c,t);
    T=C_T(c,t);
    Ptot=C_P(c,t)+Pinn;
    Ctot=Ptot/R/T;
    A[0]=0.614;
    A[1]=1.99e5;
    A[2]=8.39e5;
    E[0]=0.;
    E[1]=98.;
    E[2]=59.5;

    for (i=0;i<=2;i++)
        k[i]=A[i]*exp(-(E[i])/(R*1.e-3)/T);

    K=k[0]/k[1];
    y_NO=C_YI(c,t,no)*den/M_NO/Ctot;
    y_NH3=C_YI(c,t,nh3)*den/M_NH3/Ctot;
    CNO=y_NO*Ctot;
    CNH3=y_NH3*Ctot;
    if ((y_NO>=1.e-10)&&(y_NH3>=1.e-10))
    {
        source=k[2]*K*CNO*CNH3/(1+K*CNH3+k[2]/k[1]*CNO);
        source=source/Av*NAS*Sa*ro;           //
        [mole/m3/s]
    }
}
```

```

    }
    else{source=0.;}

    dS[eqn]=0.;
    C_UDMI(c,t,0)=source;
    return -source*M_NH3;
    [kg/m3/s]
}

DEFINE_SOURCE(NO_rxrate,c,t,dS,eqn)
{
    return -C_UDMI(c,t,0)*M_NO;
}

DEFINE_SOURCE(N2_rxrate,c,t,dS,eqn)
{
    return C_UDMI(c,t,0)*M_N2;
}

DEFINE_SOURCE(H2O_rxrate,c,t,dS,eqn)
{
    return C_UDMI(c,t,0)*M_H2O*3./2.;
}

DEFINE_SOURCE(O2_rxrate,c,t,dS,eqn)
{
    return -C_UDMI(c,t,0)*M_O2*1./4.;
}

DEFINE_SOURCE(CO2_rxrate,c,t,dS,eqn)
{
    return -C_UDMI(c,t,0)*0.0;
}

DEFINE_SOURCE(Heat_of_rx,c,t,dS,eqn)
{
    return C_UDMI(c,t,0)*dH;
}

DEFINE_DIFFUSIVITY(D_eff,c,t,i)
{
    real Deff,T,den,centre,radius;
    real NV_VEC(xc);
    T=C_T(c,t);
    den=C_R(c,t);
    C_CENTROID(xc,c,t);
    centre=0.025;
    radius=0.003;
    if(pow(pow(xc[0]-centre,2.)+pow(xc[1],2.),0.5)<radius)
        Deff=7.68e-8*pow(T,0.6);
    else
        Deff=C_MU_L(c,t)/den;
    return Deff;
}

```