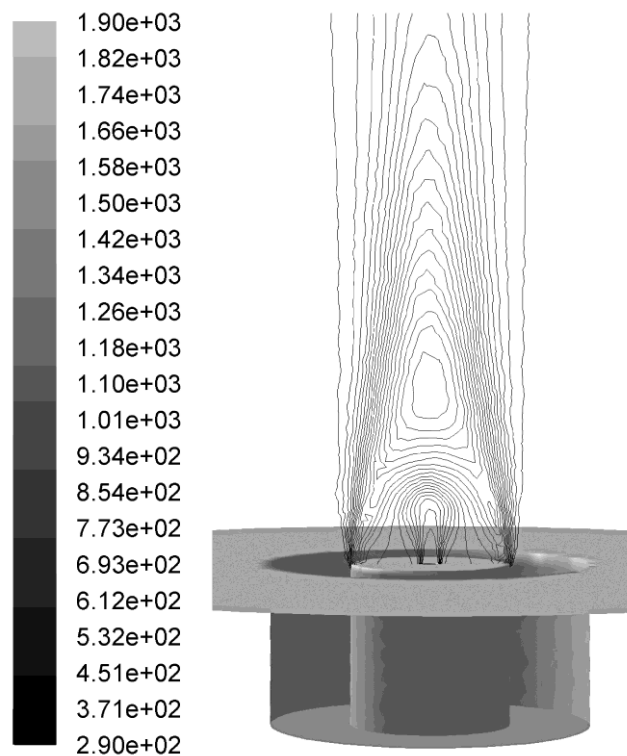

Computational Fluid Dynamics for Engineers

Tutorial 2

Non-premixed turbulent flame

Temperature [K]



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

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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 all required 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 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 do post-processing. All instructions are written for Ansys Workbench 13 and the software used are: Design Modeler, Meshing Platform, Fluent respectively.

In this tutorial a *bluff-body stabilized non-premixed turbulent flame* is studied, using the mixture fraction/PDF and equilibrium chemistry models described in Chapter 5. The purpose is that you, in accordance with best-practice guidelines, Chapter 7, learn how to:

- *Generate*: CAD and mesh files for the system (2D-axisymmetric model).
- *Analyze*: Mesh quality
- *Define*: Inlet, outlet, wall boundary conditions, turbulence model, mixture fraction/PDF model and species for equilibrium chemistry calculations.
- *Calculate*: Look-up table, flow field, turbulence, mean mixture fraction, mixture fraction variance, species and temperature fields.
- *Judge*: Convergence
- *Evaluate*: Numerical schemes, mesh independence.
- *Analyze*: Species composition, flame attachment and temperature, recirculation zone.
- *Discuss*: Validity of simulation results with respect to assumptions in the problem formulation, limitation with the model, possible refinements.

1.1 Tutorial problem description

The gas combustion system considered in this tutorial is shown in Figure 1. As seen here the fuel and air enters coaxially separated by a bluff body. The fuel consists of 100% methane, CH₄ and is combusted in air, 21%-molar Oxygen O₂, and 79% nitrogen, N₂.

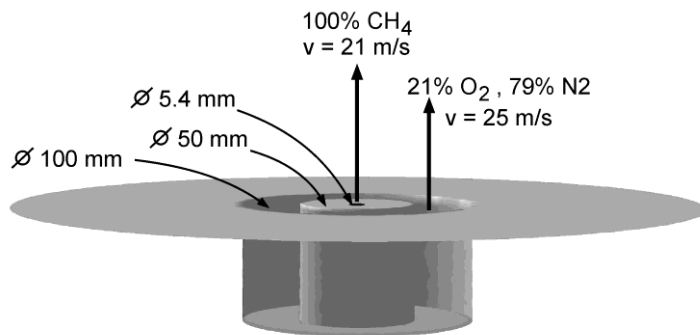


Figure 1. Schematic view of the burner (you generate a 2D-axisymmetric analysis to reduce the computational time).

Temperature measurement for the same geometry and boundary conditions simulated in this tutorial, are found in:

J. Warnatz, U. Maas, R.W. Dibble, 2006, *Combustion - Physical and Chemical Fundamentals, Modeling and Simulation, Experiments, Pollutant Formation.*, Springer. Figure 14.8.

This measurement data allows the accuracy of simulations to be judged. You are strongly encouraged to compare the measured values to the simulated ones. This book is found as an e-book on most university libraries so you can easily get access to the data.

The turbulent flame is modeled using the mixture fraction/PDF modeling approach which is based on solving transport equations for conserved scalars, i.e. mixture fraction and variance. Turbulence-chemistry interaction is modeled using a beta-function PDF. Several chemical species, radicals and intermediates in the combustion process can be included, e.g. CH₄, N₂, O₂, CO, CO₂, H₂O, NO, NO₂, CH₂O, H₂O₂, O, H, OH etc. These compounds are calculated from the predicted mixture fraction and assumption of chemical equilibrium. Create your model according to the drawing in Figure 2, and use boundary conditions given in Table 1. Note all dimensions are in millimeter.

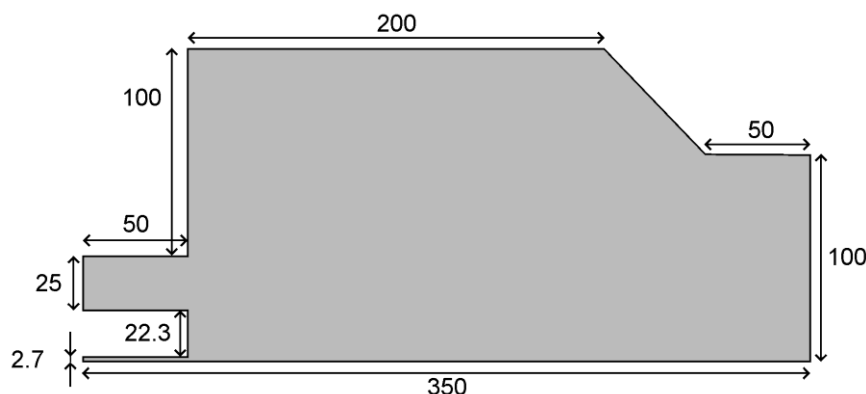


Figure 2. Drawing of the 2D-axisymmetric model.

Table 1. Boundary conditions.

| | Fuel inlet | Air inlet | Comment |
|---------------------------|----------------------|---------------------------------------|----------------|
| Velocity | 21 m/s | 25 m/s | |
| Turbulent intensity | 10% | 10% | |
| Turbulent length scale | 0.001m | 0.01m | |
| Mean mixture fraction | 1 | 0 | |
| Mixture fraction variance | 0 | 0 | |
| Species composition | 100% CH ₄ | 21%O ₂ , 79%N ₂ | Molar fraction |

Boundary conditions for the inlet can be set to velocity inlet, outlet to pressure outlet.

Boundary conditions on the walls: no-slip, zero heat flux.

The axis should be defined as rotational symmetry not regular symmetry line, since the intention is to model a coaxial flow of two gas streams.

1.2 Tutorial prerequisites

It is recommended that you have read Chapters 1-5 in the text book (*Computational Fluid Dynamics for Engineers*) and solved Tutorial 1. 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. However, steps already explained in Tutorial 1 are not shown with screen dumps. 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.

2. Tasks and report instructions

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

- What does the Damköhler number describe? (Hint Equation 5.4)
- Why is the PDF needed to calculate the reaction rate for some reactions? (Hint Chapter 5.5)
- What do the mean mixture fraction and the mixture fraction variance describe, and how do they affect the shape of the PDF? (Hint Figure 5.5)
- How is the PDF obtained in the CFD simulation? (Hint Figure 5.11)
- Calculate the degree of segregation, I_s , (Equation 5.18) and show how the mixing progresses throughout the system. (Hint: Fluent users can use Custom Field Functions to define I_s and plot it.)
- Are the boundary conditions for turbulence at the inlet appropriate? (Hint Best practice guidelines, Chapter 7 in the textbook)
- How far into the system does the turbulent boundary conditions affect the simulation results? (Hint: Estimate this using Table 4.1 in the textbook.)
- Two cold gas streams of methane and air are mixed, is it reasonable that they just start to combust?
- Which converged solution (in simulation loop nr 1-3) is the best one? How good is that prediction? Judge this based on the measurement data in, J. Warnatz et al., *Combustion - Physical and Chemical Fundamentals, Modeling and Simulation, Experiments, Pollutant Formation.*, 2006. Springer. Figure 14.8.

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.

Simulation loop nr 2

Try two approaches 1.) make the overall mesh denser in the meshing program and 2.) make an adaption after finishing Loop nr 1 using gradient adaption, i.e. refining the mesh where it is most needed (e.g. gradient of mixture fraction). (Hint: When you do mesh adaption you can view the new mesh at each time you modify it. In Ansys/Fluent it is done Display->Mesh)

- Is the number of nodes different?
- What is the difference between these results? Does the flame temperature and shape change? In that case how much does it change?

Adapt the mesh using y^+ adaption on the nozzle walls.

- How these changes affect your solution?

Use a higher order discretization scheme.

- How does the solution/results change? Why?

Simulation loop nr 3

Go back to 'Design Modeler' and change the geometry:

- decrease the inlet pipe dimension from 50 mm to 5 mm and
- decrease the outlet channel length from 50 mm to 5 mm.

Update the computational mesh. Run simulation to convergence.

- How does these changes affect your solution? Why?

Exercise

In order to show how the mixing progresses, and how the presumed PDF (beta-PDF) looks like during different stages in mixing, calculate the beta-PDF at a few different locations downstream the inlets. Use the CFD data and relevant equations in the textbook (Hint: Chapter 5.4.2).

Hint: It is not critical exactly where you select your conditions. But it is recommended that the locations are significantly separated from each other in downstream location. It is enough to select 3 different locations. You can do this plot easily in Matlab.

Optional questions (-physics of combustion)

- Can ignition of the two gases be simulated with modified model using CFD?
- What physics is lacking in the current model?
- What ignition source would be required?
- How is the minimum ignition energy (MIE) affected by flow and turbulence? Could this be predicted by CFD simulations?
- Does the CFD model account for the fuel specific flammability limits?
- Determine the stoichiometric mixture fraction (reaction $\text{CH}_4 + 2\text{O}_2 \rightarrow \text{CO}_2 + 2\text{H}_2\text{O}$).
- What is a appropriate fuel rich flammability limit? What limit has been used in your simulations? How does a change in this limit affect the solution? How does equilibrium calculations in the CFD simulations change in regions where the fuel/air compositions is above the fuel rich flammability limit?

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

The basic CAD operations where explained in Tutorial 1. Please refer to Tutorial 1 if you need to refresh your memory.

1. Start Work bench and a new project.
2. Mark Geometry->Properties/Advanced Geometry Options/Analysis Type *change to 2D*
3. Open **Design Modeler** (select to generate your model in millimeter).
4. Go to Sketching/Settings/Grid mode and *mark the check boxes: 'Snap (to grid)', 'Shown in 2D'*
5. Select the global coordinate system z-axis, to view the x-y plane.
6. In the menu select the x-y plane and add 'New sketch' (remember that symmetry axis must be aligned with the x-axis)
7. Sketching /Draw, use Polyline and make a rough* drawing as shown in Figure 2 and Figure 3 below (Start in origo with P snap. Use close end by right-clicking before you close the loop).

* you will later specify the exact dimensions according to Figure 2.
8. Sketching/Dimensions/General, define dimensions , specify the dimensions according to Figure 2.

Hint: specify the dimension in a logical order, otherwise the lines may be distorted and cross each other, also avoid making the sketch over-constrained.

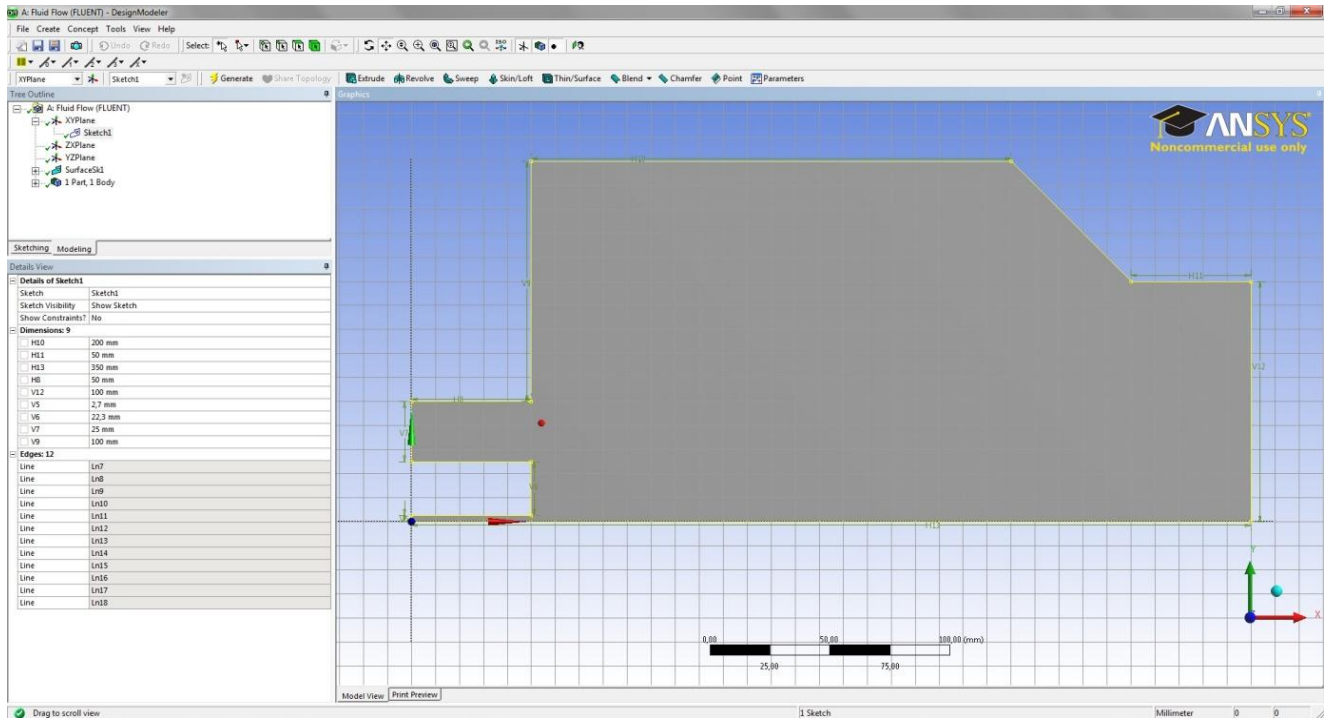


Figure 3. CAD model and dimensions.

Select the modeling tab to generate a surface based on the sketch.

10. Concepts/Surfaces from sketch, Select the sketch you just generated and push Generate

You should now have 1Part/1Body with the right dimensions and it should look like Figure 3 and 4.

11. Save the project

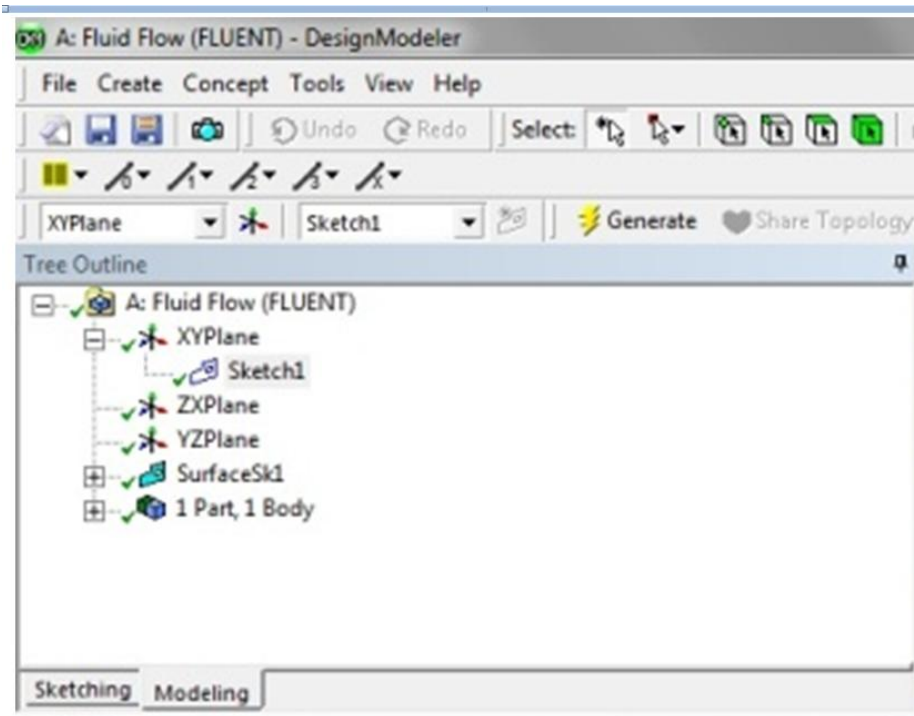


Figure 4. CAD model.

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

The basic Meshing operations where explained in Tutorial 1. Please refer to Tutorial 1 if you need to refresh your memory.

1. Start the Meshing program
2. Insert 'Inflations' , Right-click on Mesh->Insert->Inflation. Select the 2D model and the edges to which your inflations should be added. Set appropriate values for first layer thickness and growth rate under inflation options.
3. Sizing: On Proximity and curvature
4. Mark enties and group them into 'Named Selection', (Right-click on the entity, Create Named Selection, Give names -e.g. fuel_inlet, air_inlet, nozzle_walls, outer_walls, axis, outlet). To select more than one line to a specific group use Ctrl-key.
5. Define the relevance center and relevance. You may need to repeat steps 5-7 a few times to get an acceptable mesh.
6. Generate the Mesh.
7. Try modifying a few settings (maximum number of layers etc) and generate a new mesh.
8. Evaluate the mesh quality in terms of near-wall-resolution, cell skewness etc. The mesh should be acceptable but it is not critical at this point since you later will do mesh adaption and evaluate if you have a mesh-independent solution. Your mesh should look similar to Figure 5.
9. Save.

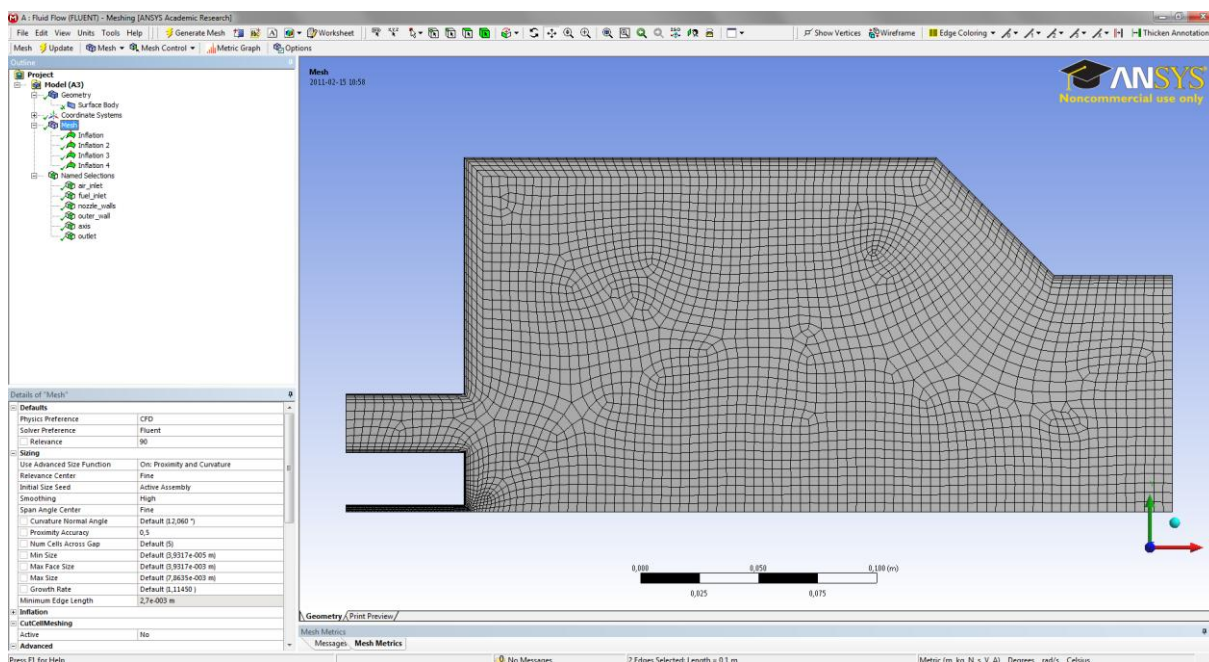


Figure 5. Computational mesh.

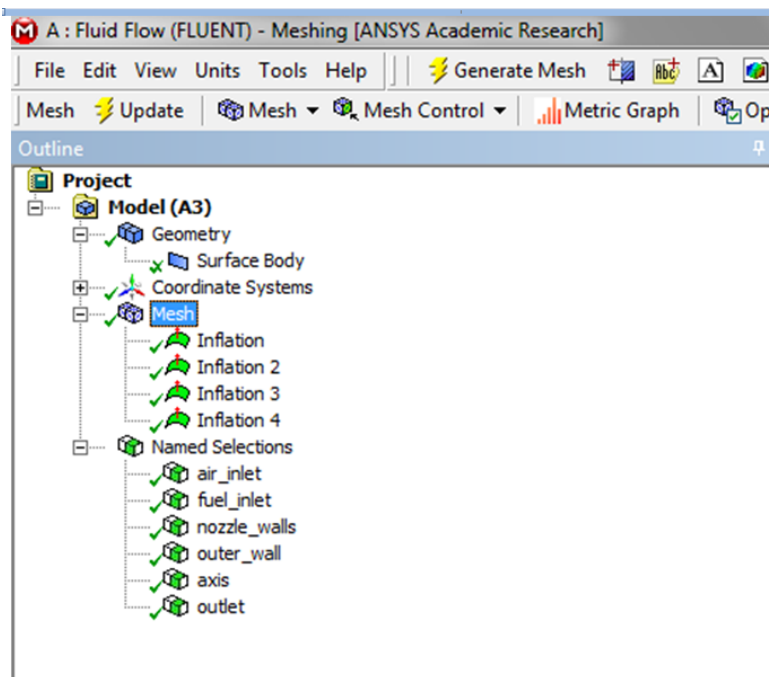


Figure 6. Mesh details.

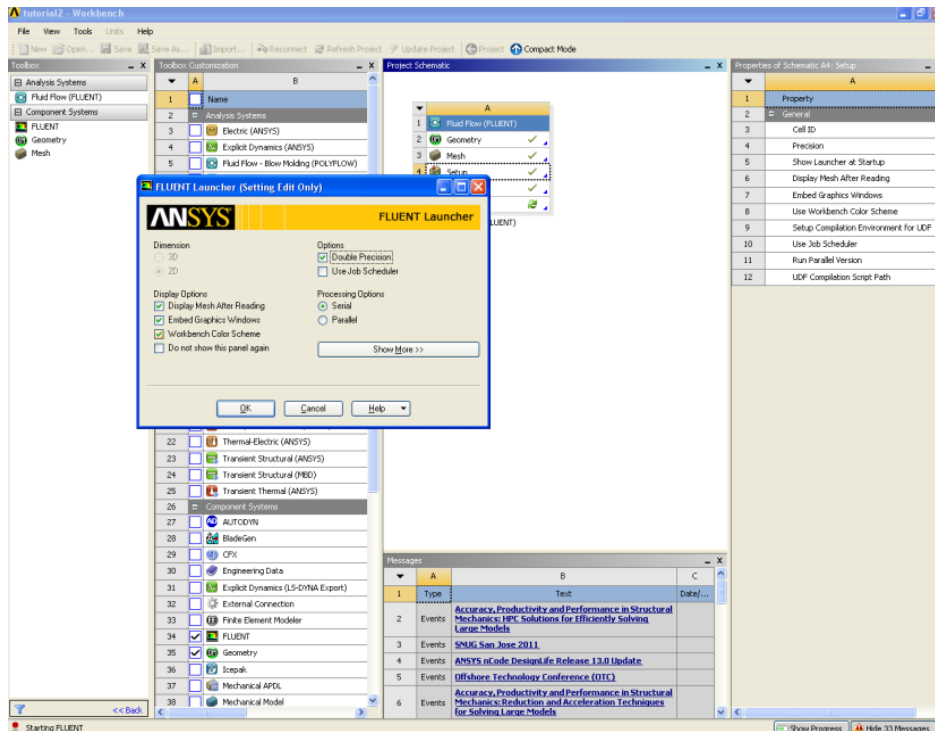
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Computational Fluid Dynamics for Engineers, Cambridge University Press, 2011.

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

The basic Fluent operations were explained in Tutorial 1. Please refer to Tutorial 1 if you need to refresh your memory.

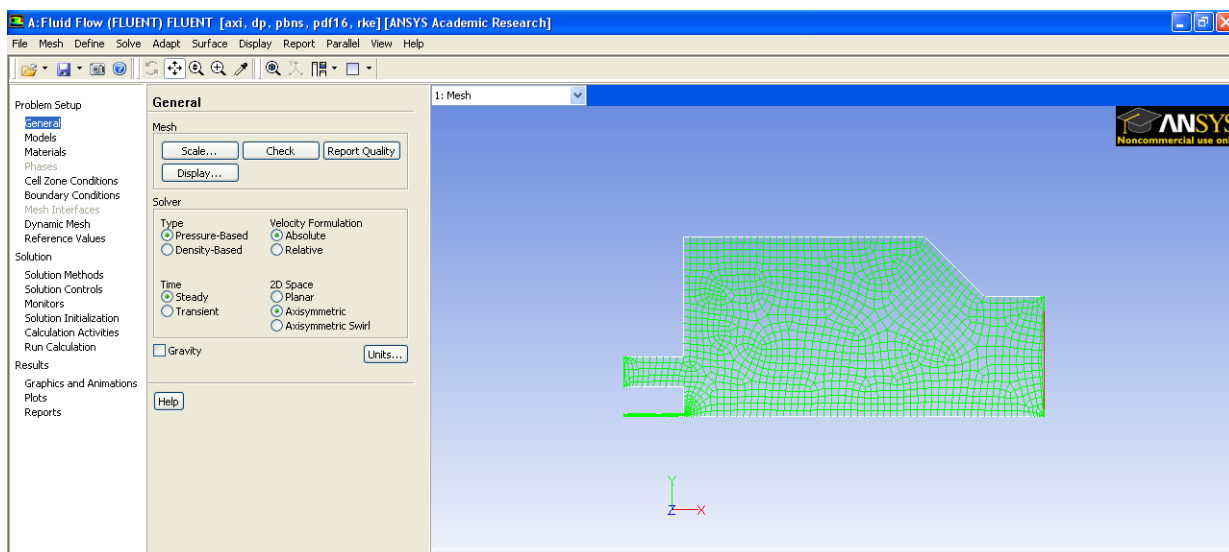
1. Start Fluent in Double precision, 2D, Serial processing.



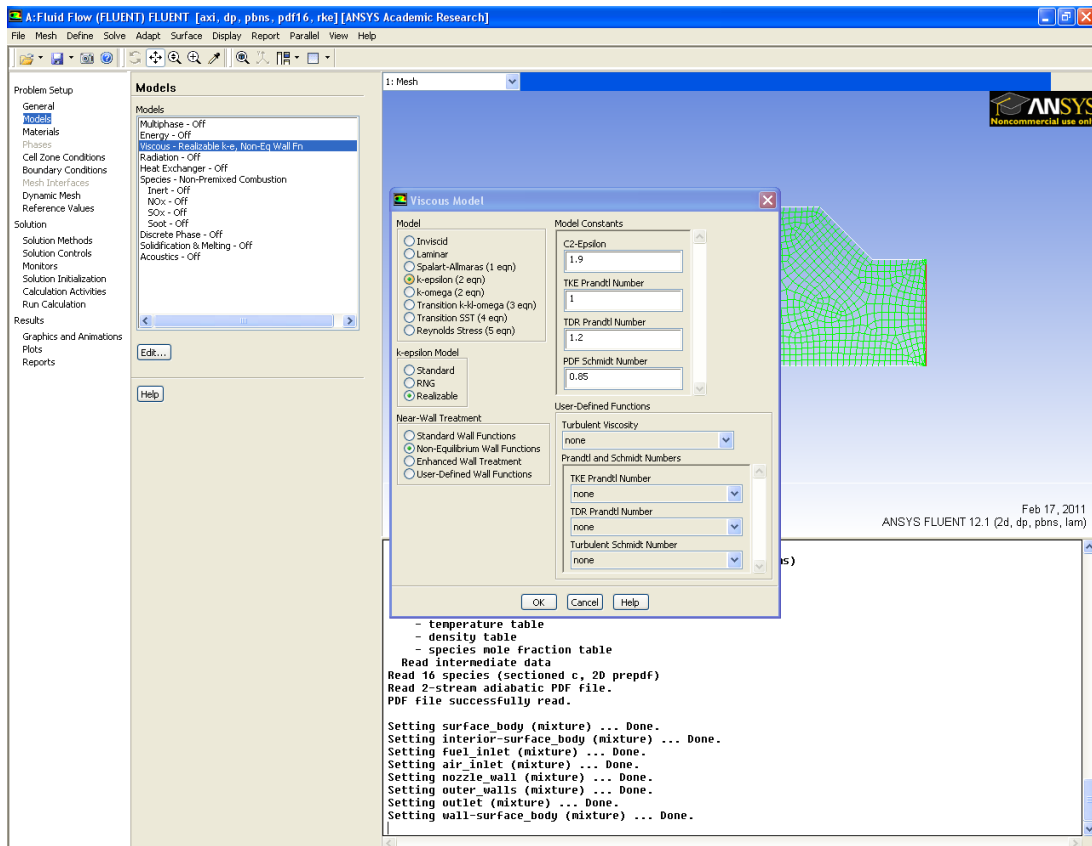
2. Check that the dimensions are correct (otherwise these can easily be changed inside Fluent if necessary, using scaling). You can also take a look at the mesh information. **Mesh\Check** and **Mesh\Info**

Define the model

3. General 2D space, *change to axis-symmetric*



Define turbulence model

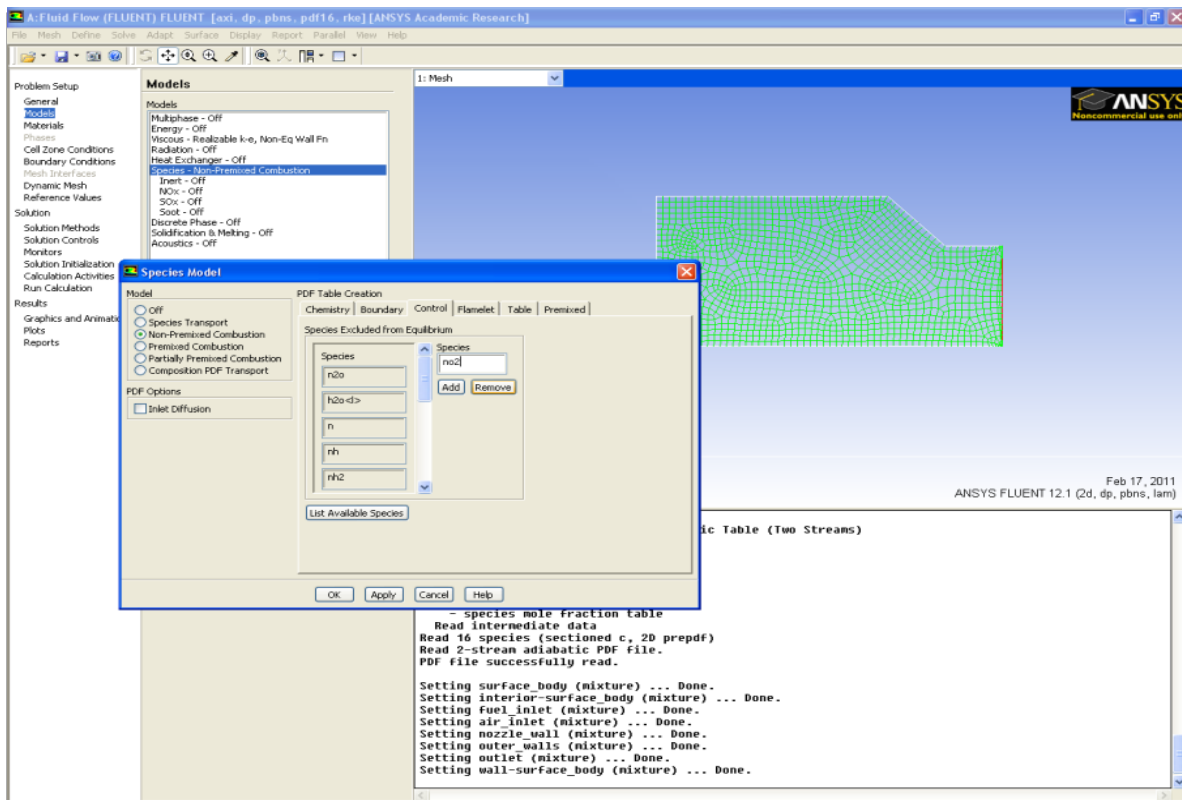
4. Models->Viscous->k- ϵ , realizable, non-eq wall functions

5. Models->Species->Select non-premixed combustion and go through each 'Tab' (shown in the Figure below)

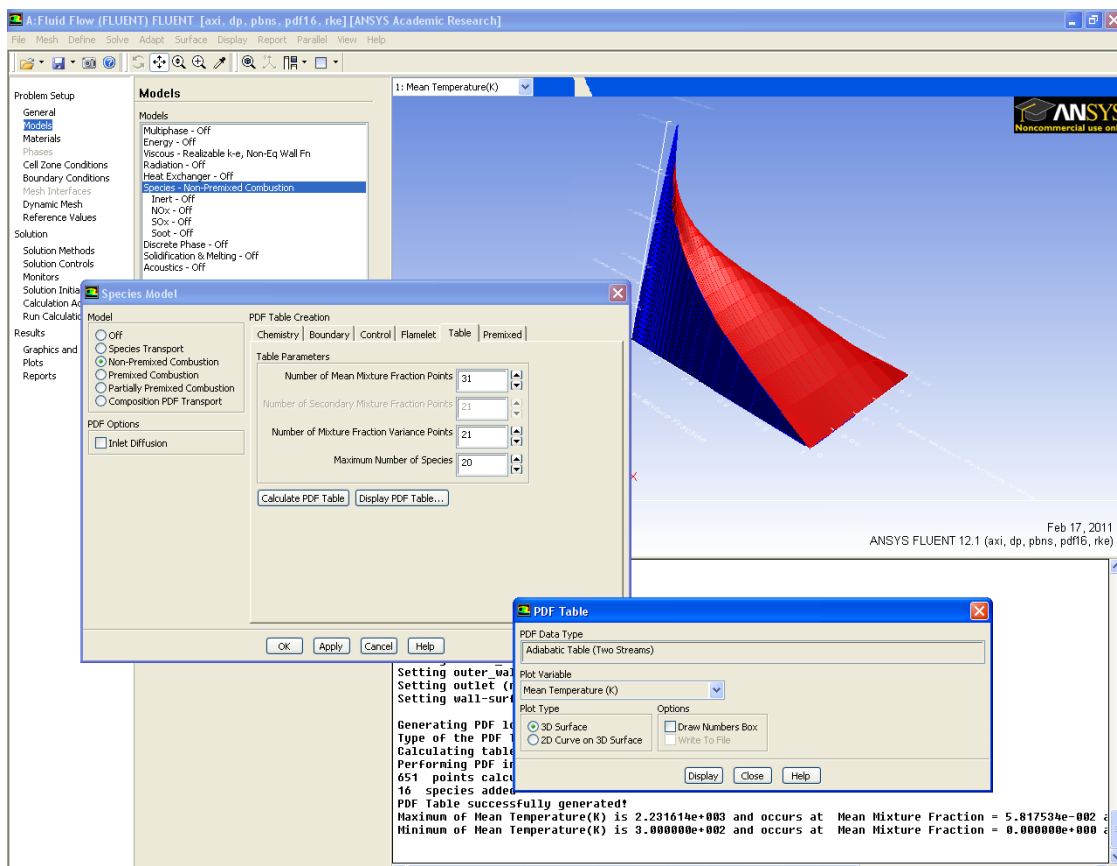
- ✓ Chemistry: Adiabatic/non-adiabatic (start with adiabatic and in loop 2 test non-adiabatic)
- ✓ Boundary: *change* to molar fraction, set CH₄ molar fraction to 1 for fuel.
- ✓ Control: Remove NO and NO₂ from excluded list (so that it gets included)

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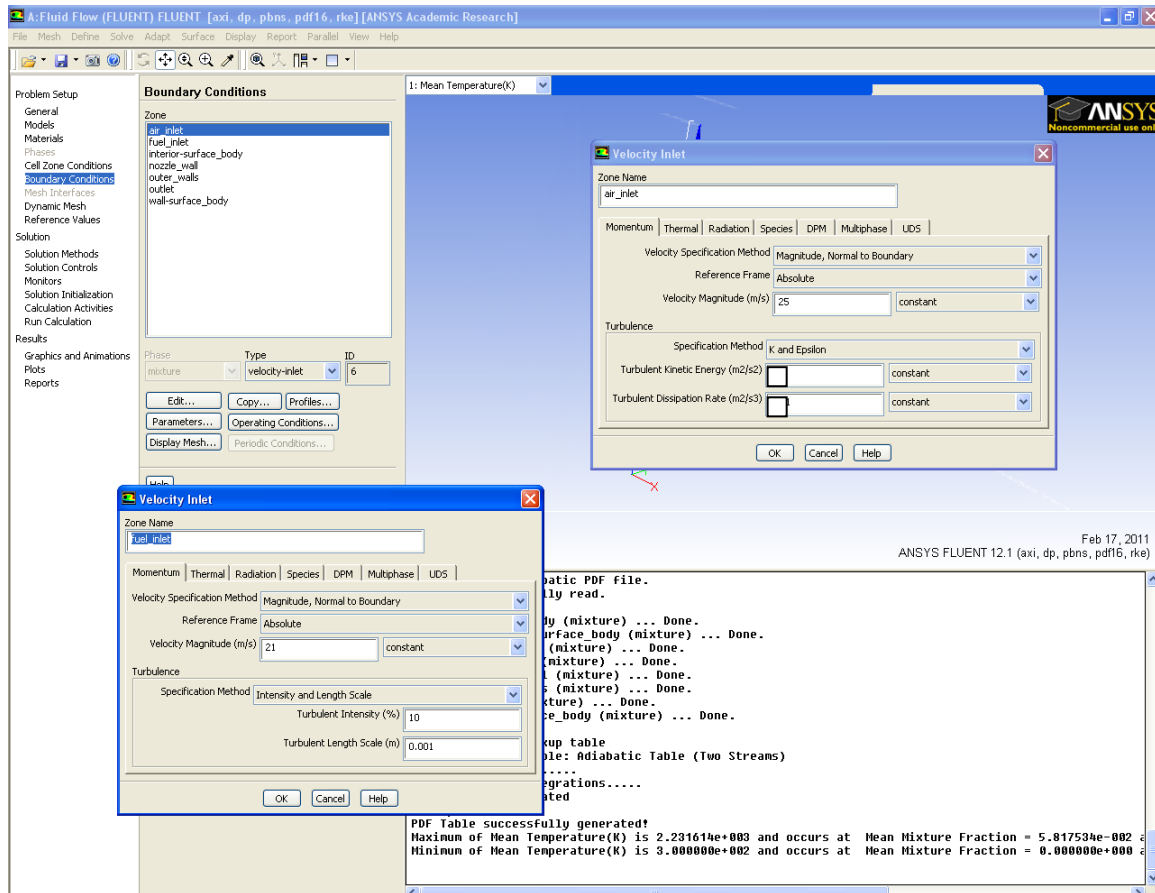


- ✓ Table: Calculate PDF table, View table(you can rotate the surface using the mouse) (see Figure below) Click Apply and OK.



6. Define the boundary conditions according to Table 1.

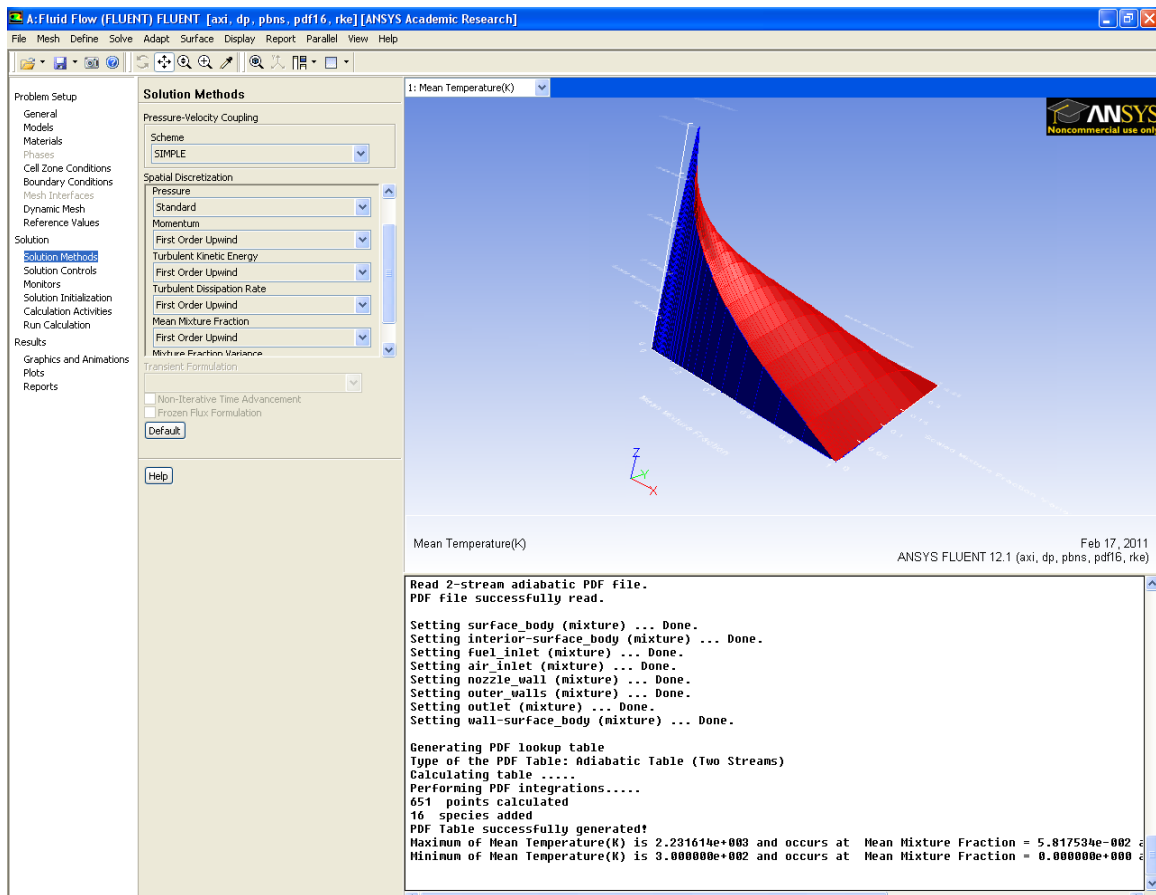
Note: for turbulence use turbulent intensity and length scale.



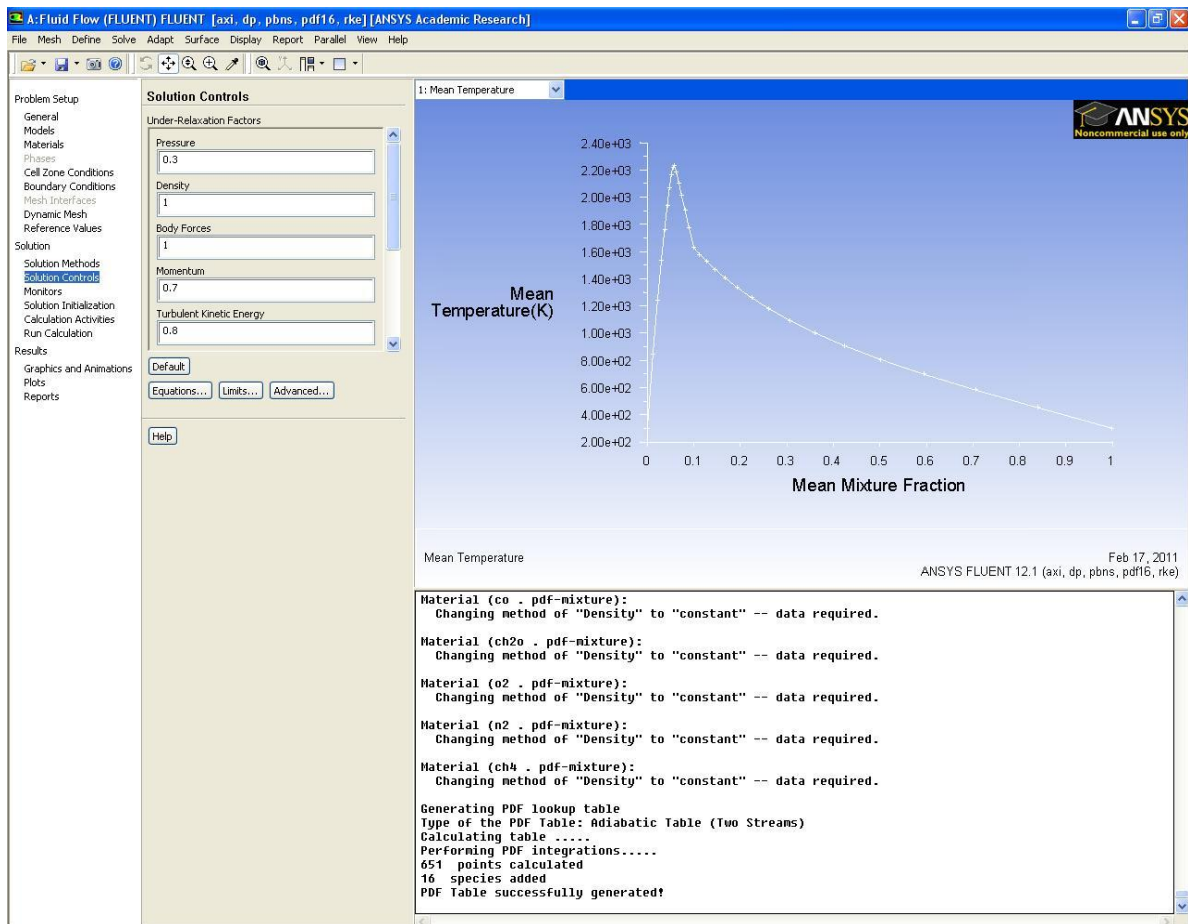
7. Solution Methods / retain the default settings and change them later to higher order scheme

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8. Solution Controls/ retain the default values for under relaxation factors to start with, modify them later if required.



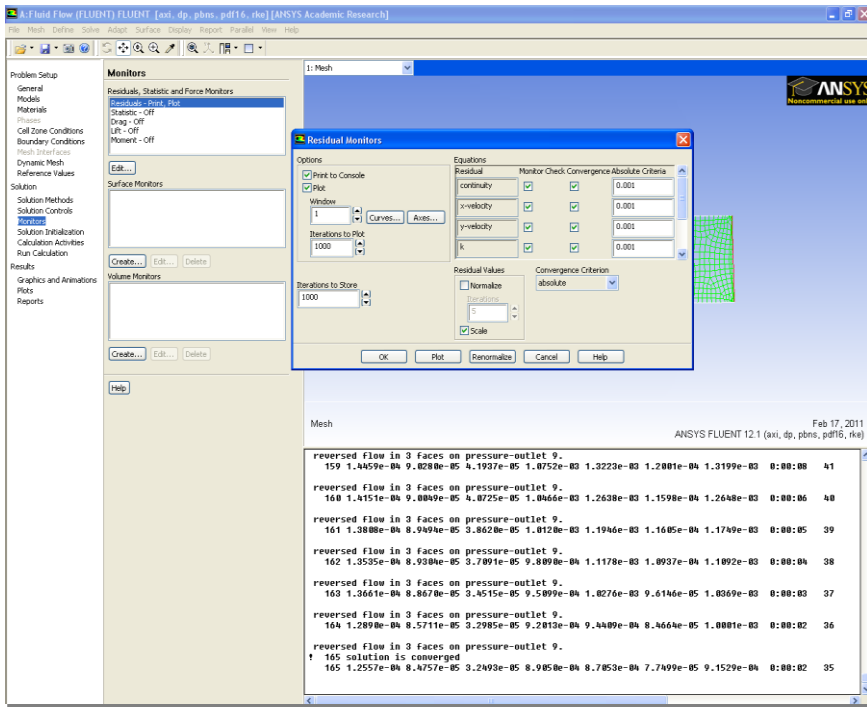
Before you start simulations you need to initialize the solution

9. Solution Initialization, Initialize

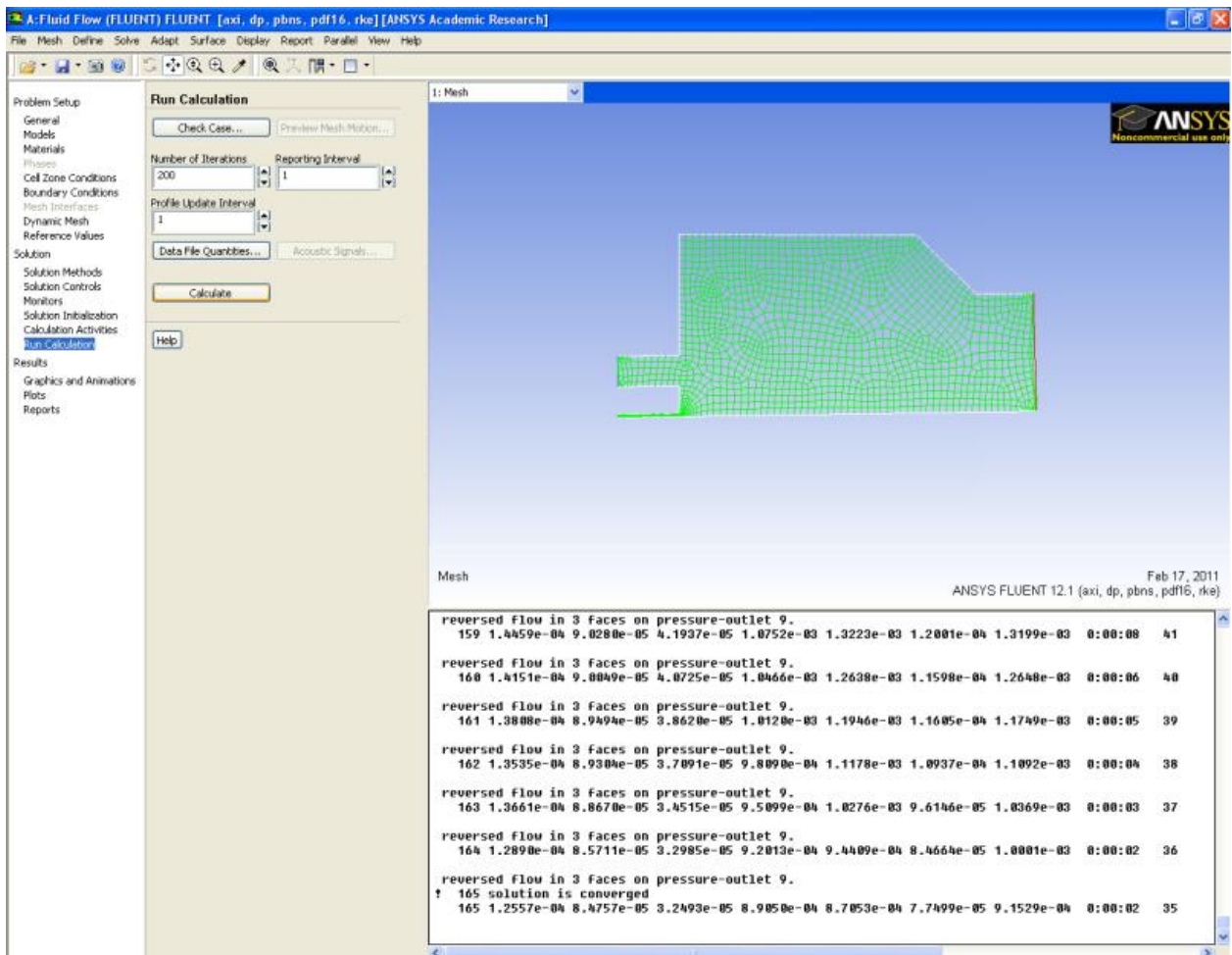
Solve/Monitor/residual Edit-> / you can accept the default values and may add new monitors you find useful.

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10. Run Calculation, these simulations will reach convergence very fast, typically within one minute.

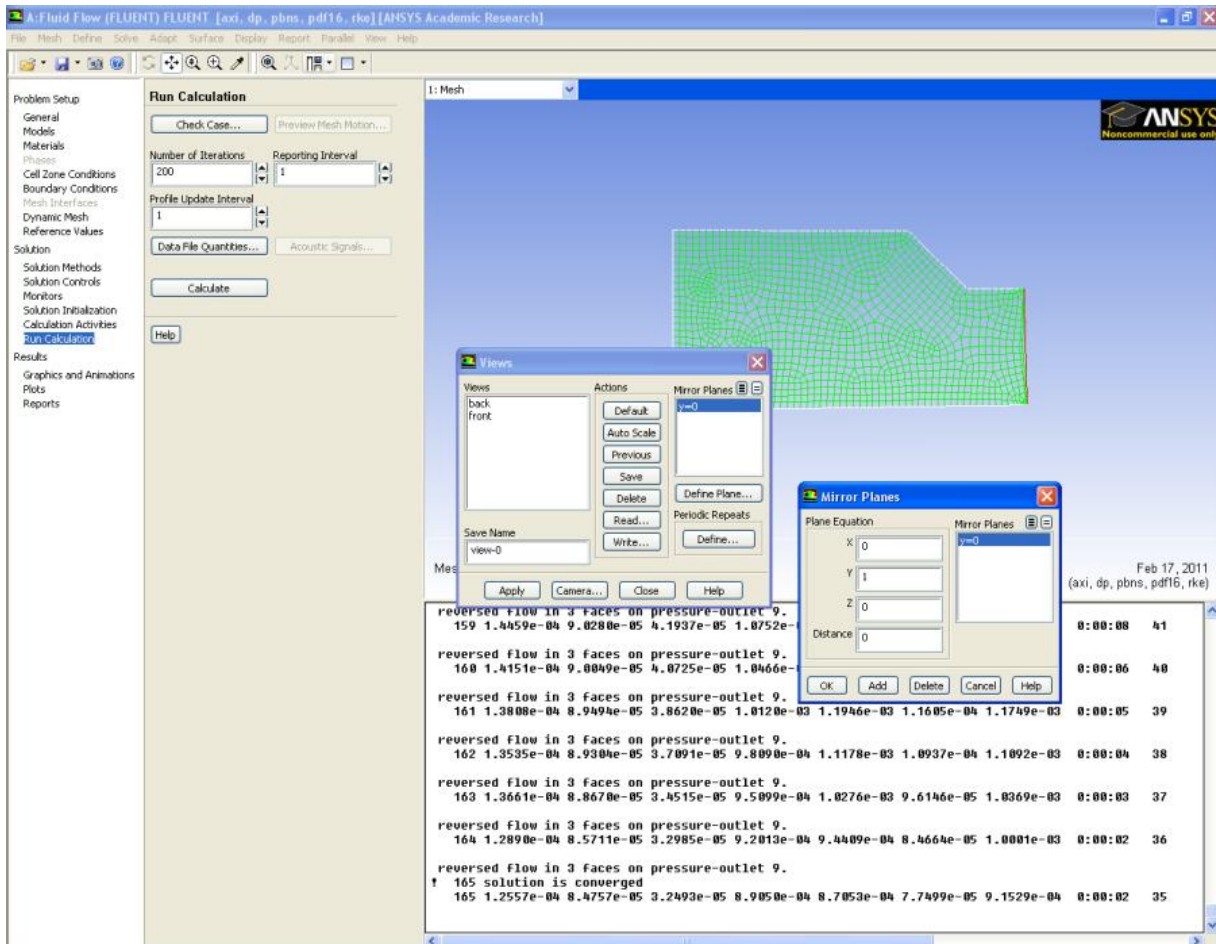


You can modify the view by mirror the computational domain using the symmetry axis.

11. Display/Views/Mirror planes (select your symaxis) Click Apply. Rotate the view if you prefer to see the flame vertically.

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Analyze: Mean Mixture fraction, mixture fraction variance, temperature, species composition. Plot vector field, look for recirculation.

Hint: You can use scaling factors on vectors to make certain zones more clear.

