Tutorial: Modeling Liquid Reactions in CIJR Using the Unsteady Laminar Flamelet Model

Introduction

The purpose of this tutorial is to demonstrate setup and solution of liquid chemical reactions using the unsteady laminar flamelet model in ANSYS FLUENT.

Reactions in liquid typically display slow chemical kinetics and low species diffusivity (or high Schmidt number). Slow chemistry implies that fast chemistry models of ANSYS FLUENT, such as the non-premixed equilibrium model, steady laminar flamlet model, and the eddy-dissipation model cannot give accurate results. Low molecular diffusion especially for reactors at low Reynolds number, causes slow mixing and high species variance. Finite-rate chemistry models, in particular the laminar finite-rate and eddy dissipation concept (EDC) model of ANSYS FLUENT do not rigorously account for the turbulence-chemistry interaction and may not predict conversion, selectivity, and scale-up accurately. The PDF transport model can handle both the finite-rate chemistry and the low diffusivity of the species, but the computational cost involved is very high since kinetic calculations are performed using particle based methods (Monte-carlo methods) which are computationally intensive.

This tutorial demonstrates how to do the following:

- Set up liquid chemical reactions in a confined impinging jet reactor.
- Set up unsteady laminar flamelet model with liquid micro-mixing extension.
- Import a CHEMKIN mechanism.
- Calculate a solution for steady and unsteady flamelet models.
- Examine results using graphics.

Prerequisites

This tutorial is written with the assumption that you have completed Tutorial 1 from ANSYS FLUENT 14.5 Tutorial Guide, and that you are familiar with the ANSYS FLUENT navigation pane and menu structure. Some steps in the setup and solution procedure will not be shown explicitly. A good understanding of turbulence and species mixing/reaction, as well as their modeling is desirable.

Problem Description

The unsteady laminar flamelet model is able to account for both the slow chemistry and the reduced mixing due to the low diffusivity. It also offers significant reduction in run time by reducing stiff kinetic calculations to one dimension. This tutorial solves for the following set of liquid kinetics occurring in bulk species in a confined impinging jet reactor.

$$A + B \rightarrow P_1$$

$$A + D \rightarrow P_2$$

The first reaction is very fast, and the second is very slow. When the liquid micro-mixing model is enabled, ANSYS FLUENT assumes that the activation energy for the reaction is small, so reaction proceeds immediately after mixing. A diagram of the CIJR with two reactants impinging at the center of the reactor is shown in Figure 1.

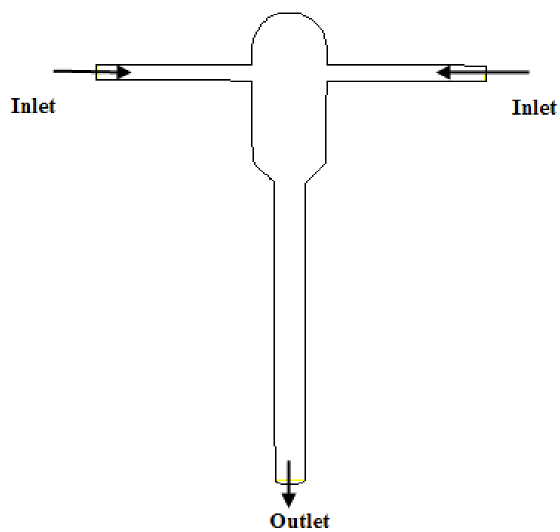


Figure 1: Problem Schematic

Setup and Solution

Preparation

1. Copy the files (`CIJR.msh.gz`, `CIJR.che`, and `CIJR-therm.dat`) to your working folder.
2. Use FLUENT Launcher to start the 3D version of ANSYS FLUENT.
3. Enable Double-Precision in the Options list.

   Ensure that the Display Options *are enabled. Therefore, after you read in the mesh, it will be displayed in the embedded graphics window.*

Step 1: Mesh

1. Read in the mesh file (`CIJR.msh.gz`).

   File ⟶ Read ⟶ Mesh...

   As the mesh file is read, ANSYS FLUENT *will report the progress in the console.*

Step 2: General Settings

1. Retain the default solver settings.

   General

2. Check the mesh (see Figure 2).

   General ⟶ Check

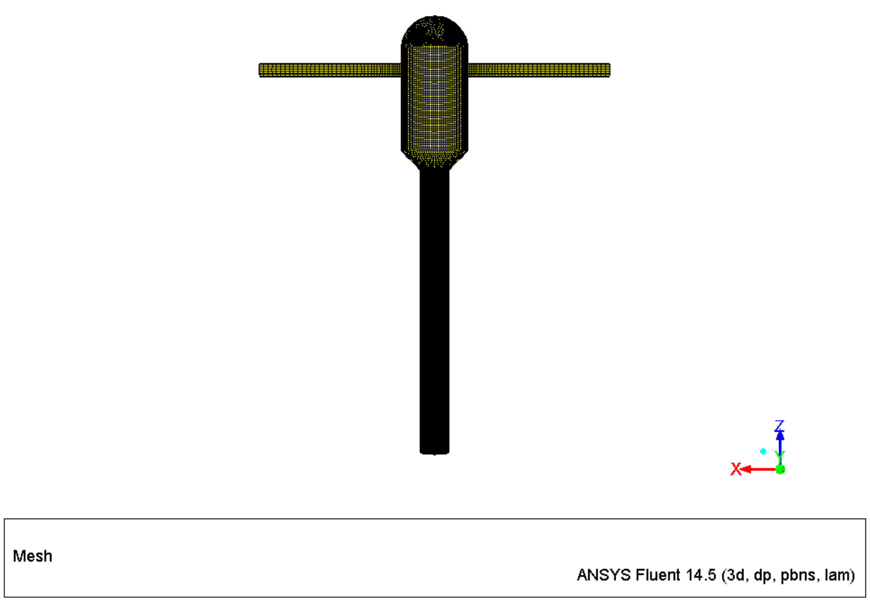
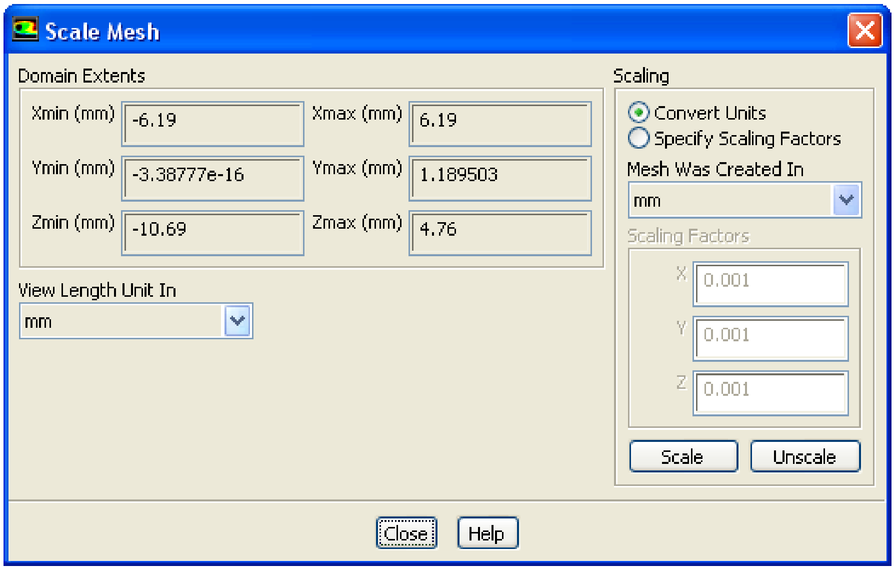


Figure 2: Mesh

ANSYS FLUENT *will perform various checks on the mesh and will report the progress in the console. Make sure the minimum volume reported is a positive number.*

3. Scale the mesh.

   General ⟶ Scale...



   (a) Select mm from the Mesh Was Created In drop-down list.

   (b) Select mm from the View Length Unit In drop-down list.

   All dimensions will now be shown in millimeters.

   (c) Click Scale and close the Scale Mesh dialog box.

Step 3: Models

1. Select the realizable k-ϵ turbulence model.

   Models ⟶ Viscous ⟶ Edit...

   (a) Select k-epsilon from the Model list to open Viscous Model dialog box.

      i. Select Realizable from the k-epsilon Model list.

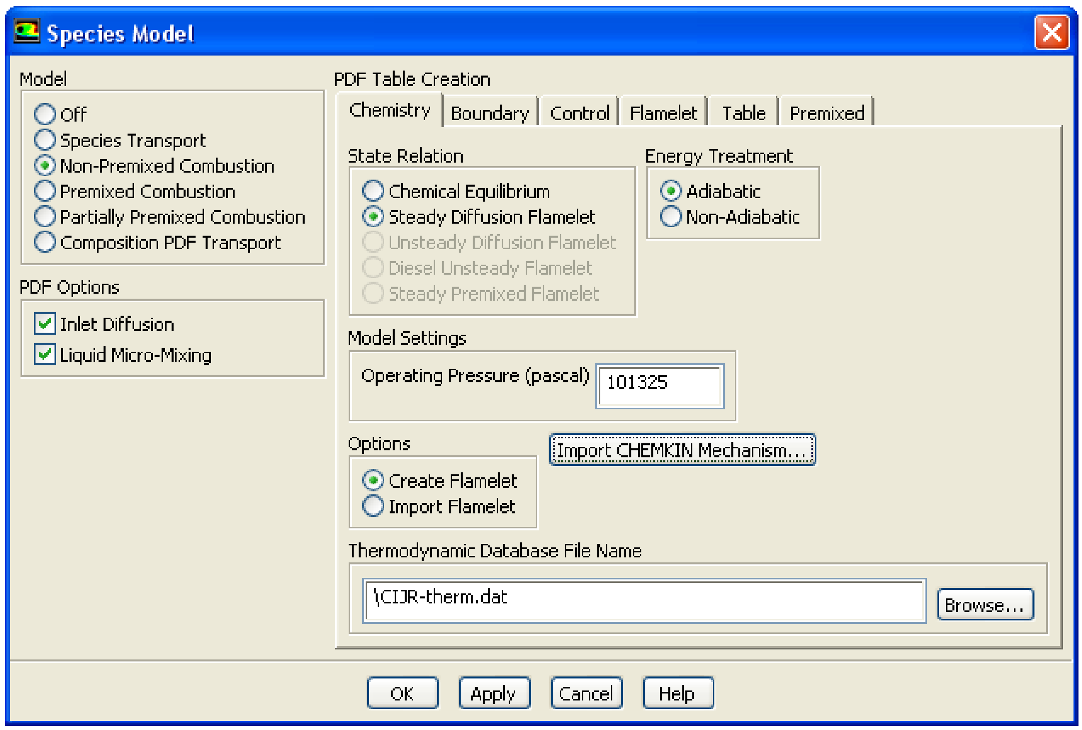
      ii. Click OK to close the Viscous Model dialog box.

Note: *The slow kinetics of CIJR requires the usage of one of the models: laminar finite-rate model, EDC model, transported PDF model, or unsteady laminar flamelet model. The first two models cannot accurately capture the micro-mixing of liquid reactions, and the transported PDF model is computationally demanding. In this tutorial you will use the unsteady laminar flamelet model with the liquid micro-mixing extension. This model requires the initial solution of a steady laminar flamelet model.*

2. Define the species model.

   Models ⟶ Species ⟶ Edit...

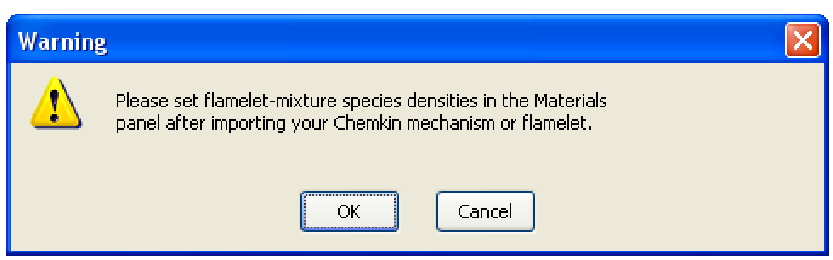
   (a) Select Non-Premixed Combustion from the Model list to open Species Model dialog box.



   (b) Select Steady Diffusion Flamelet under the Chemistry tab.

   (c) Enable Inlet Diffusion in the PDF options group box.

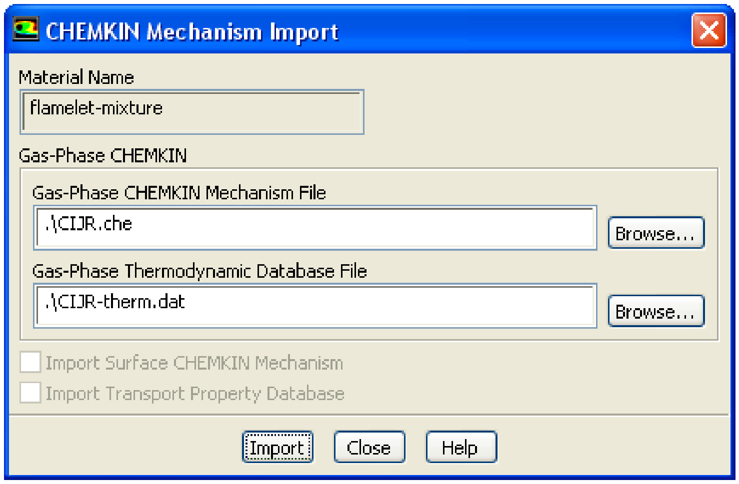
   (d) Enable Liquid Micro-Mixing in the PDF Options group box.



   (e) Click OK to close the Warning dialog box.

   At this stage, ANSYS FLUENT *requires the chemical mechanism which contains the species, their thermodynamic properties, and kinetics.*

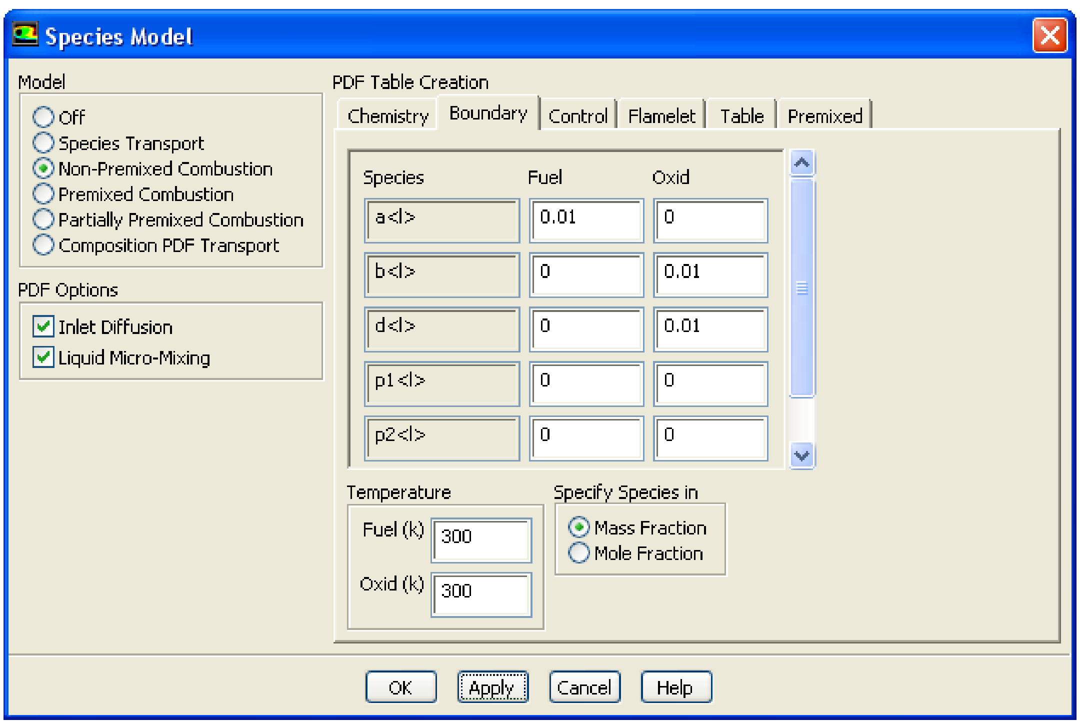
(f) Click Import CHEMKIN Mechanism... to open the CHEMKIN Mechanism Import dialog box.



i. Select `CIJR.che` for the Gas-Phase CHEMKIN Mechanism File and `CIJR-therm.dat` for the Gas-Phase Thermodynamic Database File.

ii. Click Import and then close the CHEMKIN Mechanism Import dialog box.

(g) Click Boundary tab in the Species Model dialog box.

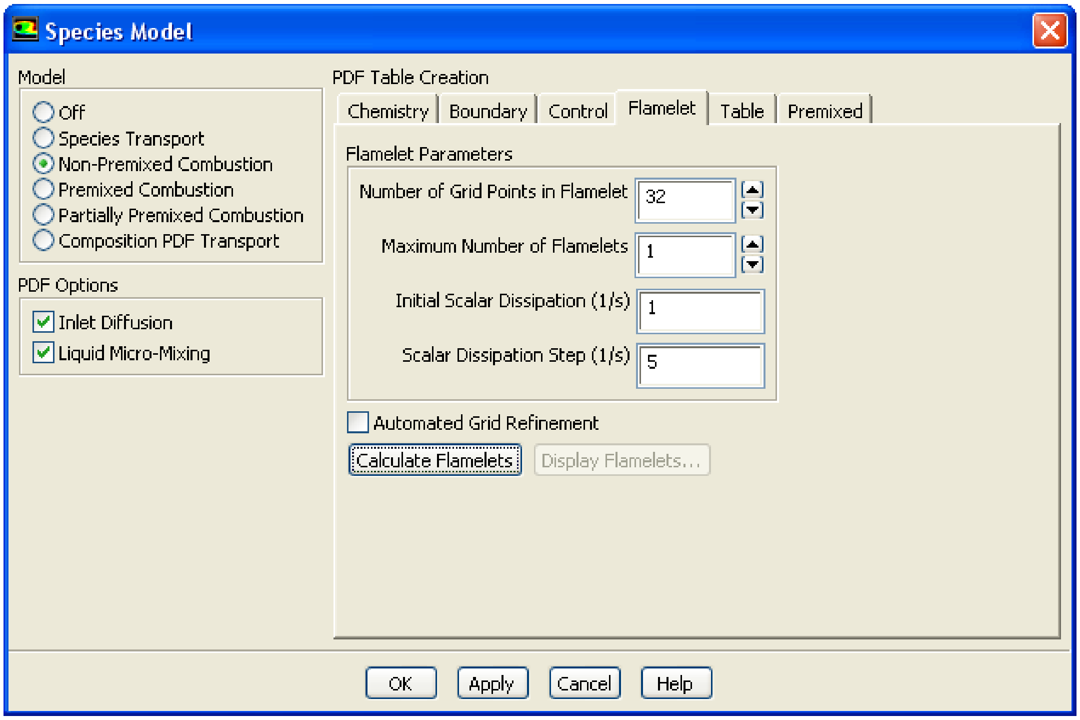


i. Enter `0.01` for a<I> and `0.99` for bulk<I> under Fuel.

ii. Enter `0.01` for b<I>, `0.01` for d<I>, and `0.98` for bulk<I> for Oxid.

iii. Click Apply.

(h) Click Flamelet tab in the Species Model dialog box.



i. Set Maximum Number of Flamelets to 1.

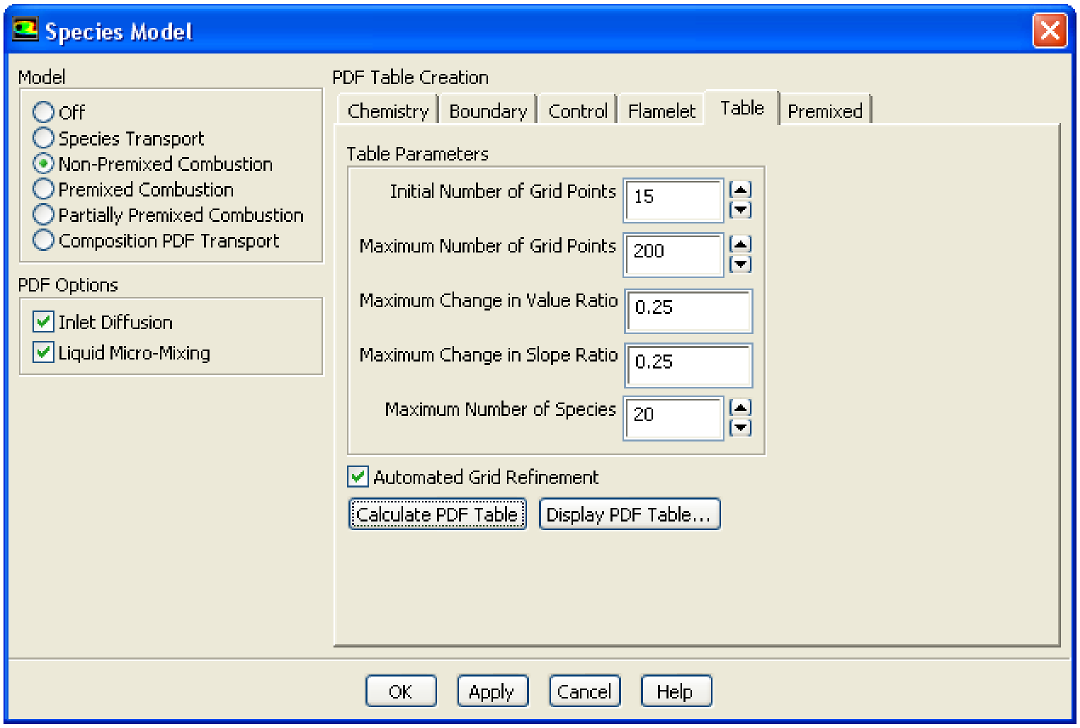
ii. Set Initial Scalar Dissipation to 1/s.

Though the steady flamelet solution is inaccurate for liquid reactions, it is required as a starting point for solving the unsteady flamelet solution. Therefore it is required to use at least one flamelet at arbitrary scalar dissipation of 1*/sec at which the steady flamelet solution can be computed.*

iii. Click Calculate Flamelets.

iv. Save the flamelet file (`CIJR.fla.gz`) after it finishes calculation.

(i) Click Table tab in the Species Model dialog box.



i. Click Calculate PDF Table.

ii. Click OK to close the Species Model dialog box.

3. Save the PDF file (`CIJR.pdf.gz`).

File ⟶ Write ⟶ PDF...

Step 4: Materials

Materials ⟶ Create/Edit...

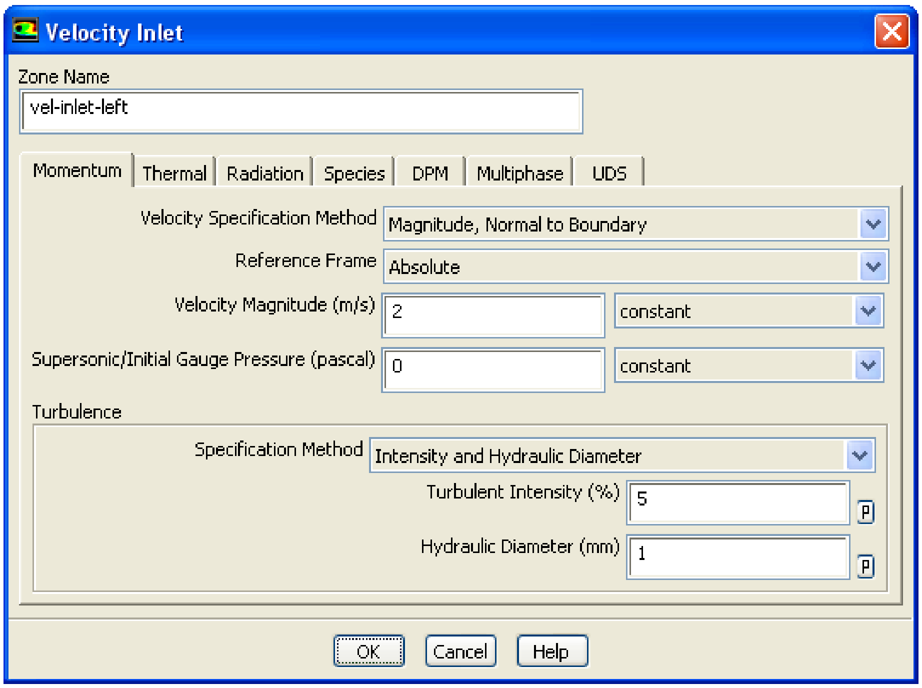
Check the pdf-mixture *and* flamelet-mixture *materials. Ensure that the density of each of the species is set to* 1000.

Step 5: Boundary Conditions

Boundary Conditions

1. Set boundary conditions for vel-inlet-left.

   Boundary Conditions ⟶ vel-inlet-left ⟶ Edit...



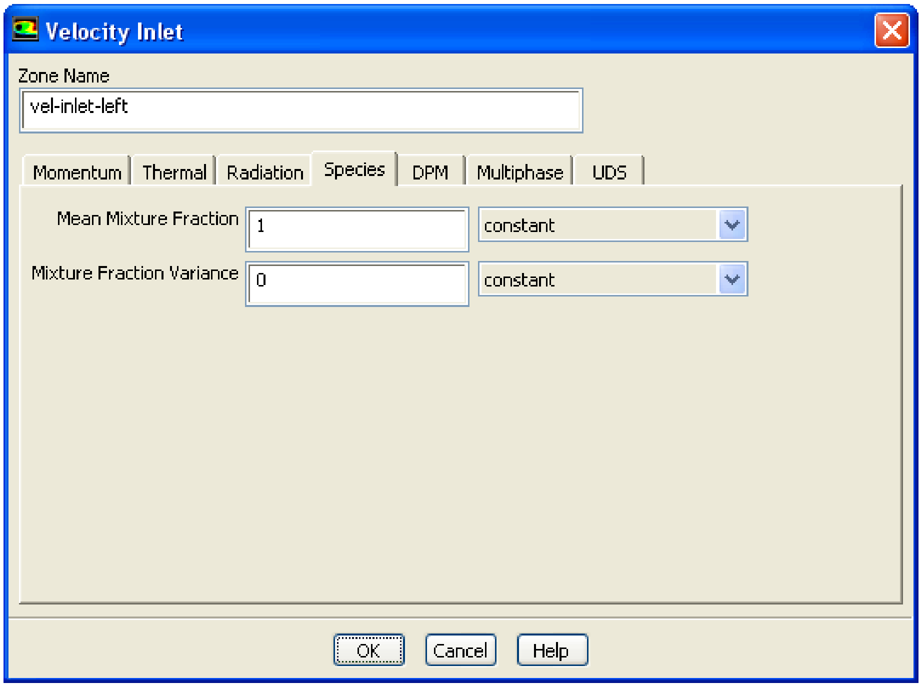
   (a) Enter 2 m/s for Velocity Magnitude.

   (b) Select Intensity and Hydraulic Diameter from the Specification Method drop-down list.

   (c) Retain 5% for Turbulent Intensity.

   (d) Enter 1 mm for Hydraulic Diameter.

   (e) Click the Species tab and enter 1 for the Mean Mixture Fraction.

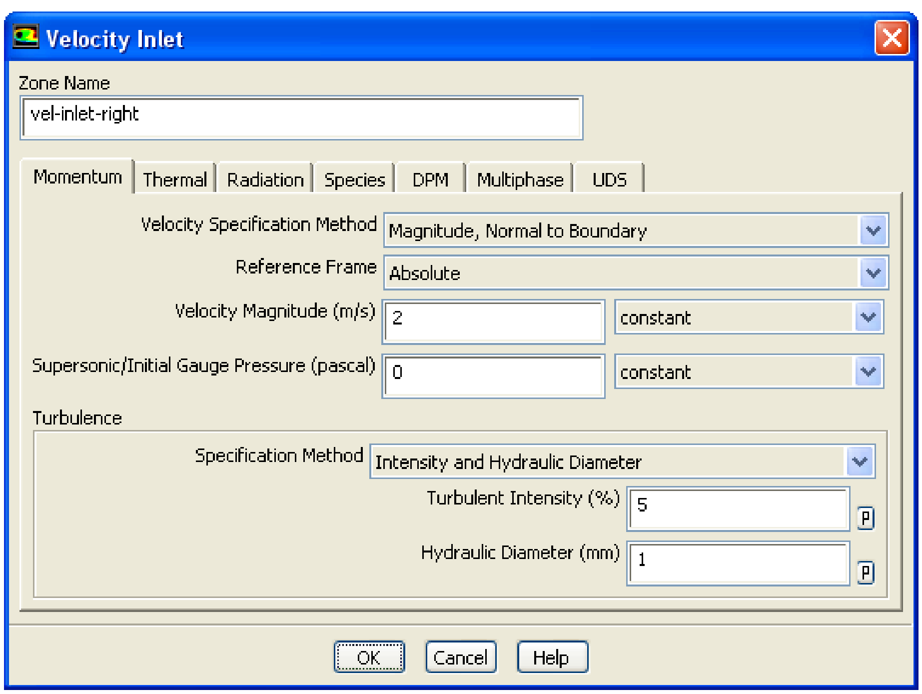


This is the 'fuel' reactant inlet, so the Mean Mixture Fraction *is* 1 *and the* Mixture Fraction Variance *is* 0*.*

(f) Click OK to close the Velocity Inlet dialog box.

2. Set boundary conditions for vel-inlet-right.

Boundary Conditions → vel-inlet-right → Edit...



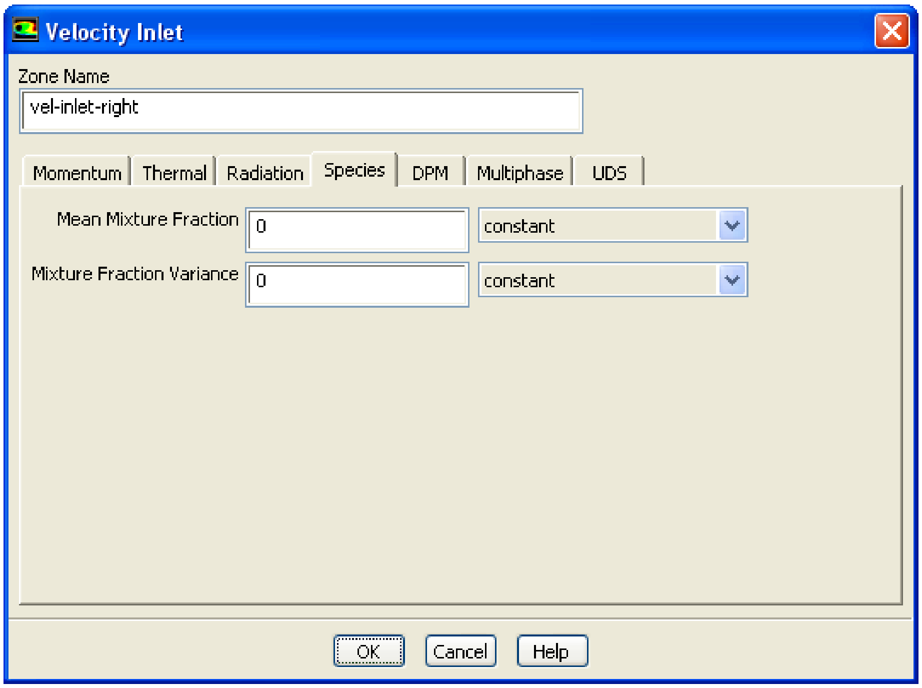
(a) Enter 2 m/s for Velocity Magnitude.

(b) Select Intensity and Hydraulic Diameter from the Specification Method drop-down list.

(c) Retain 5% for Turbulent Intensity.

(d) Enter 1 mm for Hydraulic Diameter.

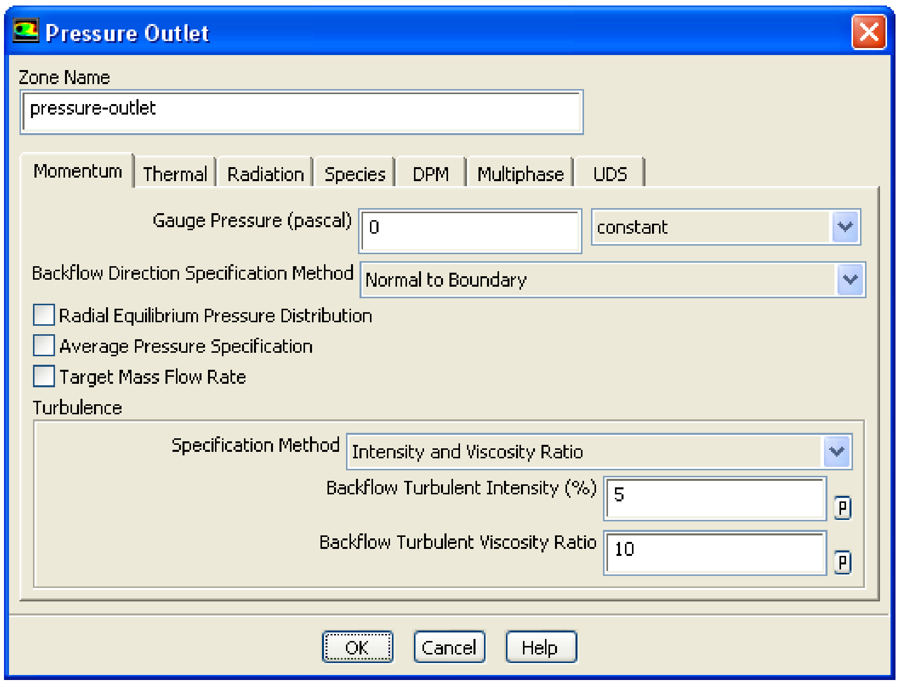
(e) Click the Species tab and retain the default value of 0 for Mean Mixture Fraction and Mixture Fraction Variance.



(f) Click OK to close the Velocity Inlet dialog box.

3. Set boundary conditions for pressure-outlet.

   Boundary Conditions ⟶ pressure-outlet ⟶ Edit...



   (a) Retain the selection of Intensity and Viscosity Ratio from the Specification Method drop-down list.

   (b) Retain 5% for Backflow Turbulent Intensity.

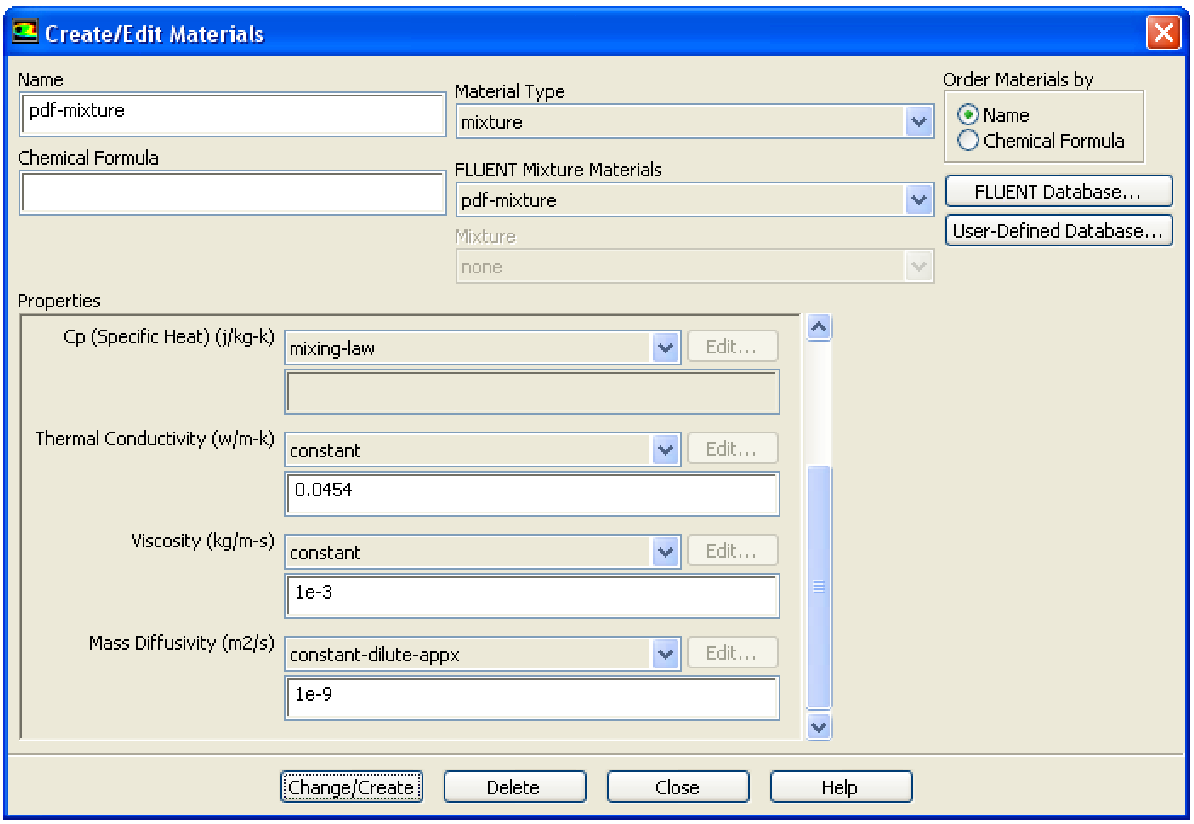
   (c) Retain 10 for Backflow Turbulent Viscosity Ratio.

   (d) Click OK to close the Pressure Outlet dialog box.

4. Set the viscosity and diffusivity of the liquid.

   The non-premixed model uses pdf-mixture *as a mixture material and you have to set the* Viscosity *and the* Mass Diffusivity *of the liquid.*

   Materials ⟶ pdf-mixture ⟶ Create/Edit...



   (a) Enter `1e-3` kg/m-s for the Viscosity.

   (b) Enter `1e-9` m2/s for the Mass Diffusivity.

   This corresponds to a Schmidt number ($Sc = \frac{Viscosity}{Density \times MassDiffusivity}$) *of* 1000.

   (c) Click Change/Create and close the Create/Edit Materials dialog box.

Step 6: Solution for Steady Flamelet Model

As the density is constant, the flow is decoupled from the mixture fraction equations. Therefore in this particular case, you can converge the simulations faster by solving for only flow and turbulence to begin with, and then you can solve for the mixture fraction equation.

1. Initialize the solution.

   Solution Initialization ⟶ Initialize

   Hybrid Initialization *is the default* Initialization Method *in* ANSYS FLUENT *14.5. Refer to the section* 28.11 Hybrid Initialization, *in the* ANSYS FLUENT *14.5 User's Guide.*

2. Save the case file (`CIJR-1.cas.gz`).

   File ⟶ Write ⟶ Case...

3. Run the calculation for 250 iterations.

   Run Calculation

   (a) Enter 250 for the Number of Iterations.

   (b) Click Calculate.

   The scaled residuals are as shown in Figure 3. The solution converges after approximately 240 iterations.

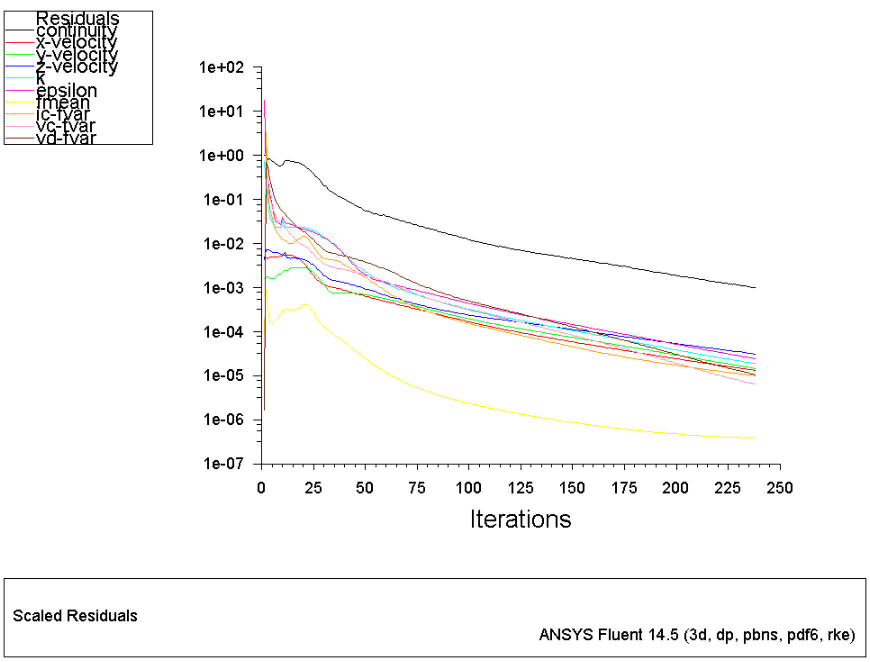


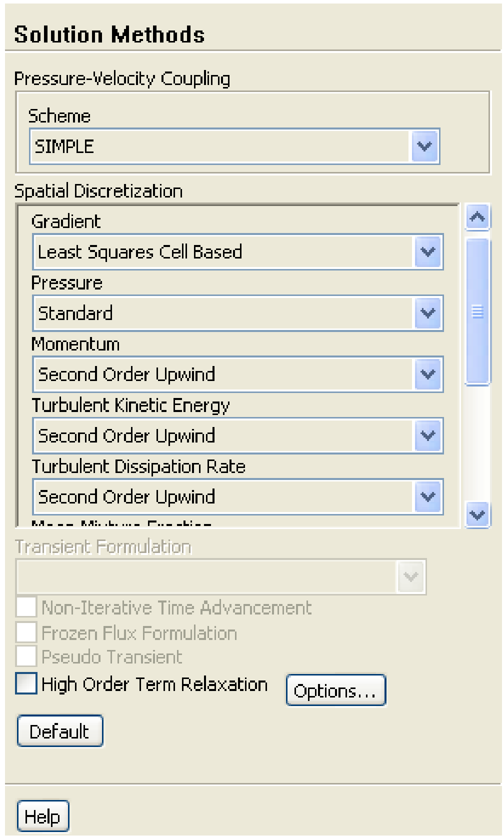
Figure 3: Scaled Residuals After 250 Iterations

4. Save the data file (`CIJR-1.dat.gz`).

   File ⟶ Write ⟶ Data...

5. Set the solution parameters.

   Solution Methods



   (a) Select Second Order Upwind for Turbulent Kinetic Energy and Turbulent Dissipation Rate.

   (b) Ensure Second Order Upwind is selected for all the parameters in the Spatial Discretization group box.

6. Save the case file (`CIJR-2.cas.gz`).

   File ⟶ Write ⟶ Case...

7. Run the calculation for 100 iterations.

   Run Calculation

   (a) Enter 100 for the Number of Iterations.

   (b) Click Calculate.

   The scaled residuals are as shown in Figure 4.

8. Save the data file (`CIJR-2.dat.gz`).

   File ⟶ Write ⟶ Data...

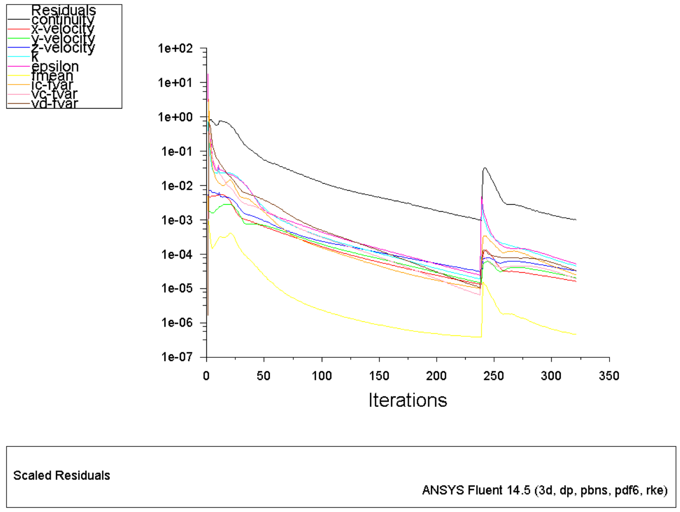
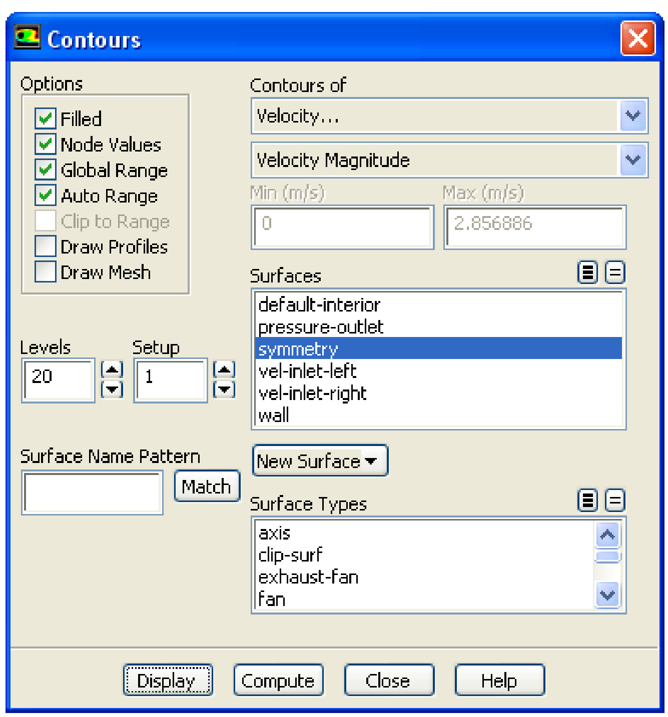


Figure 4: Scaled Residuals After Additional 100 Iterations

Step 7: Postprocessing for Steady Flamelet Model

1. Display contours of velocity magnitude.

   Graphics and Animations ⟶ Contours ⟶ Set Up...



   (a) Select Velocity... and Velocity Magnitude from the Contours of drop-down list.

   (b) Select symmetry from the Surfaces list.

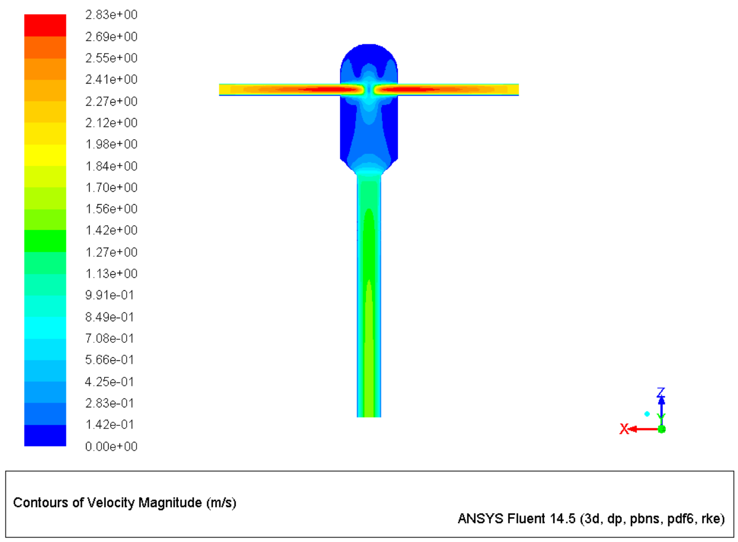


Figure 5: Contours of Velocity Magnitude

(c) Click Display (see Figure 5).

2. Display the contours of turbulent viscosity.

    (a) Select Turbulence... and Turbulent Viscosity from the Contours of drop-down list.

    (b) Click Display (see Figure 6).

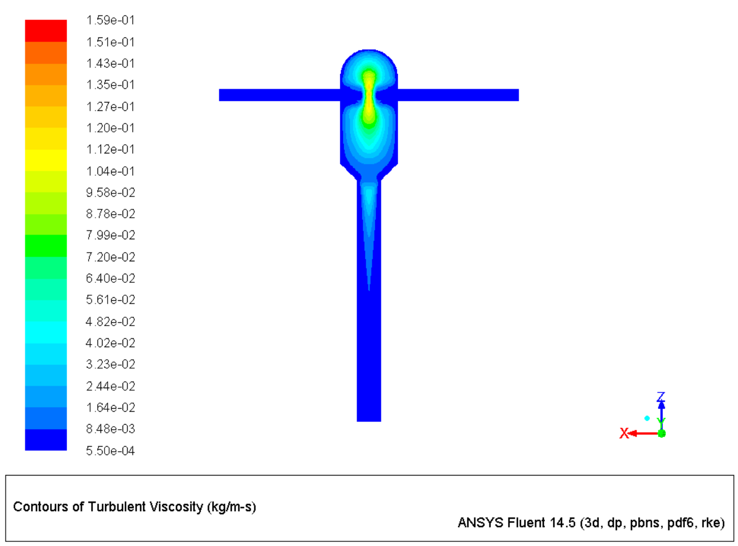
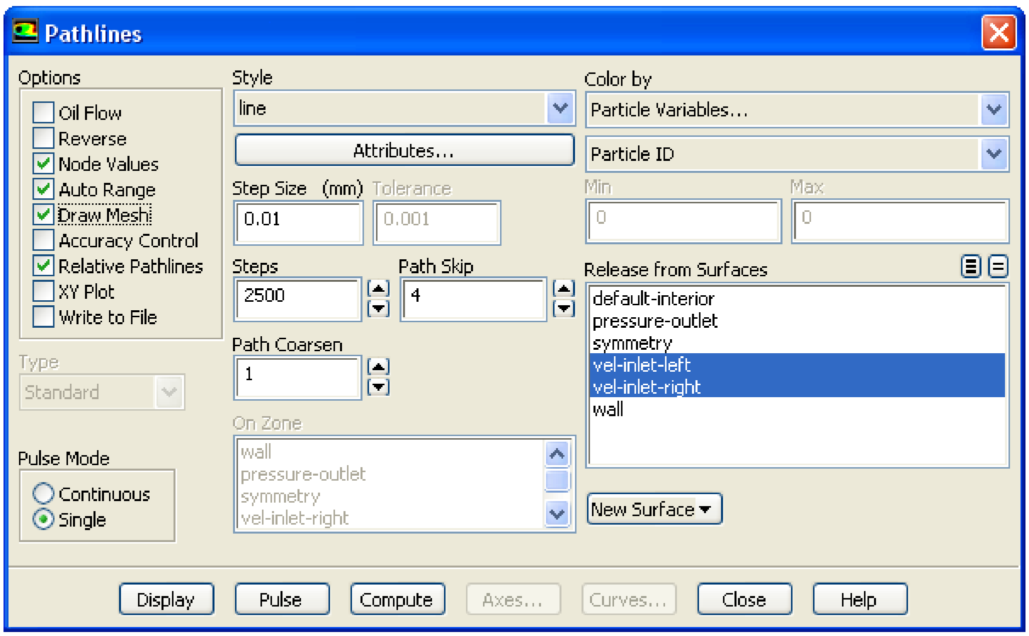


Figure 6: Contours of Turbulent Viscosity

This is indicative of the turbulence Reynolds number, which is very small.
The micro-mixing model solves transport equation for inertial-convective, viscous-convective, and viscous-diffusive subranges of the turbulent scalar spectrum. The sum of these variances is equal to the total mixture fraction variance.

3. Display the pathlines.

   Graphics and Animations ⟶ Pathlines ⟶ Set Up...



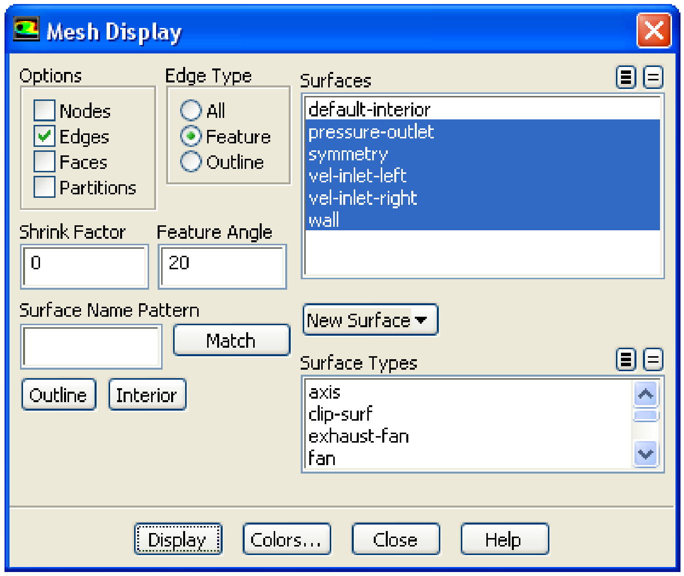
   (a) Ensure that the Step Size is 0.01 mm.

   (b) Ensure that the Steps are set to 2500.

   (c) Ensure that the Path Skip is set to 4.

   (d) Select vel-inlet-left and vel-inlet-right from the Release from Surfaces list.

   (e) Enable the Draw Mesh option.



i. Ensure that Feature is selected in the Edge Type group box.

ii. Ensure that other than default-interior all other Surfaces are selected .

iii. Click Display and close the Mesh Display dialog box.

(f) Click Display and close the Pathlines dialog box.

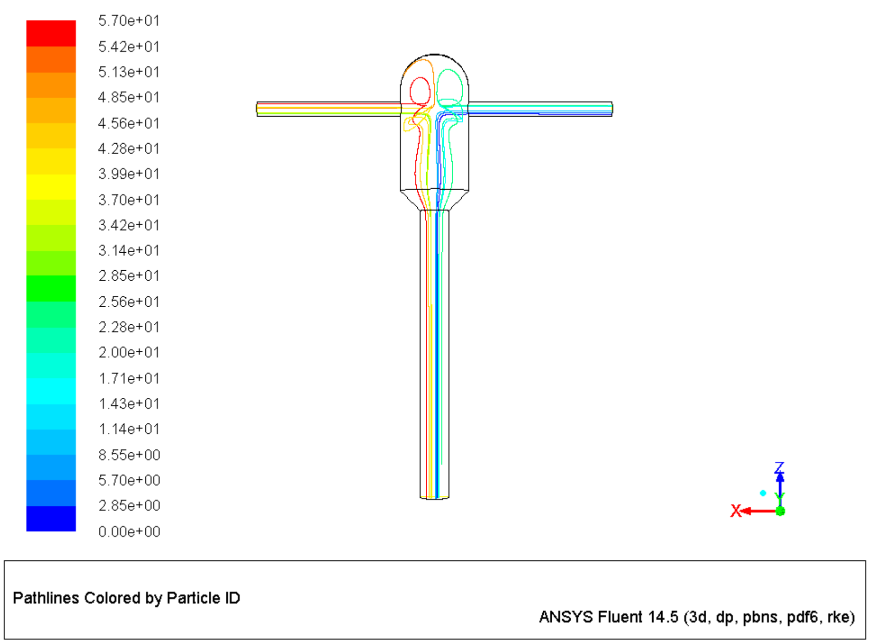


Figure 7: Pathlines

The residence time of a fluid element released at the inlet is about 0.1s.

4. Save the case and data files (`CIJRdisplay.cas/dat.gz`).

File ⟶ Write ⟶ Case & Data...

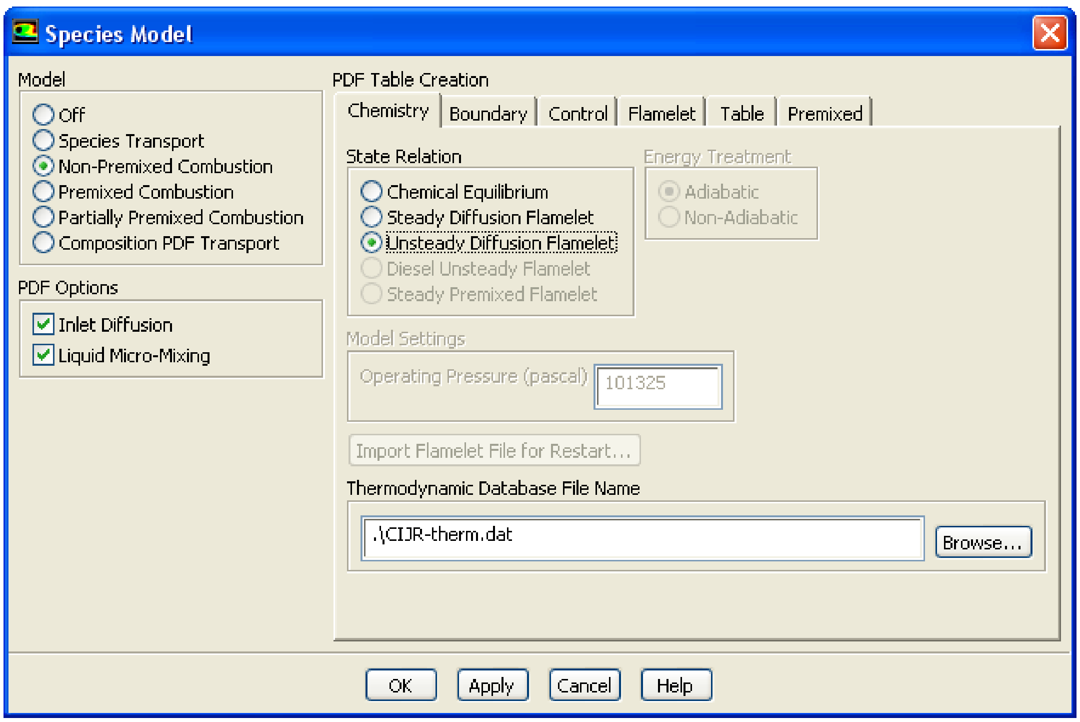
Step 8: Solution for Unsteady Laminar Flamelet Model

Solve for the species using the unsteady laminar flamelet model which is capable of capturing the slow kinetics. The unsteady flamelet model post-processes the unsteady flamelet species field on a steady state, steady flamelet ANSYS FLUENT *solution. A marker equation for flamelet probability is solved in an unsteady manner, simultaneously with the ID flamelet equations.*

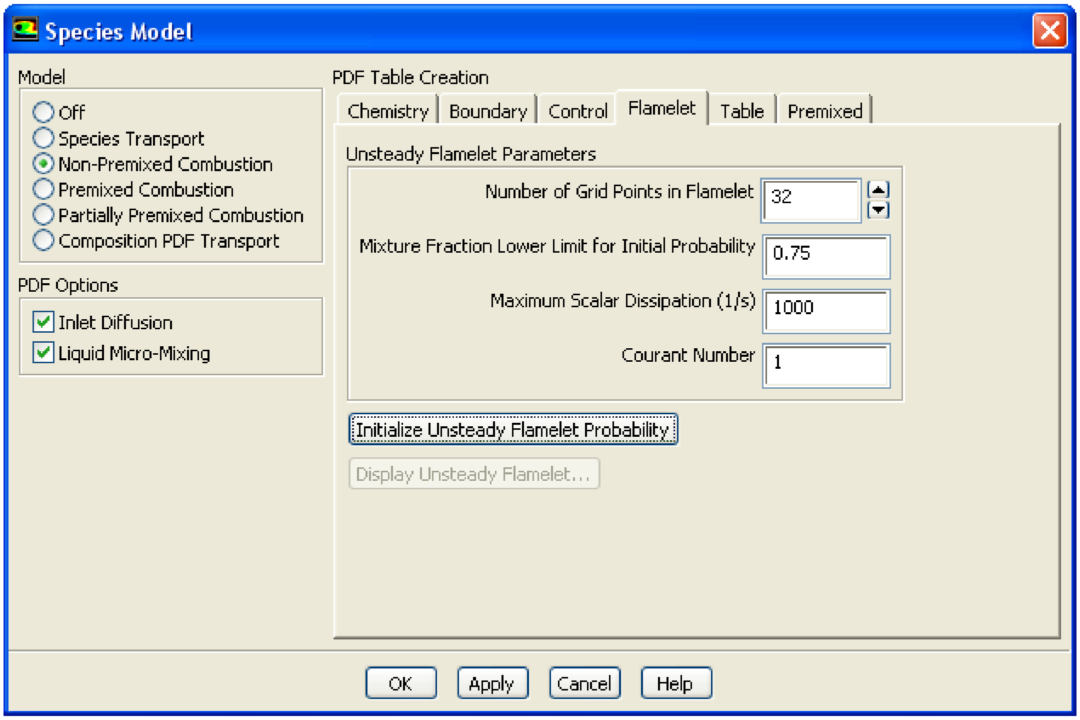
1. Define the species unsteady laminar flamelet model.

   Models ⟶ Species ⟶ Edit...

   (a) Click Chemistry tab and select Unsteady Diffusion Flamelet.



(b) Click Flamelet tab.



i. Retain the default value of Number of Grid Points in Flamelet.

ii. Enter 0.75 for the Mixture Fraction Lower Limit for Initial Probability.

The stoichiometric mixture fraction for this chemistry is 0.5. The Mixture Fraction Lower Limit for Initial Probability *should be greater than the stoichiometric mixture fraction.*

iii. Enter 1000/s for Maximum Scalar Dissipation.

The maximum scalar dissipation is an input for gas-phase flames to avoid flamelet extinction at a huge modeled strain rate. You do not require it as you are simulating liquid reactions and are not concerned with the extinction.

iv. Ensure that the Courant Number is 1.

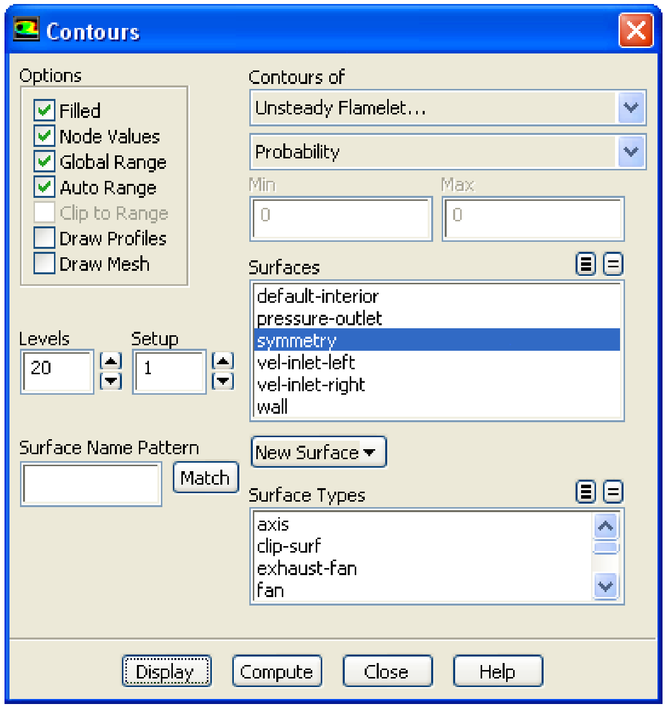
v. Click Initialize Unsteady Flamelet Probability.

The unsteady flamelet species are accumulated as the marker probability is convected and diffused out of the domain. When you click the Initialize Unsteady Flamelet Probability *button,* ANSYS FLUENT *automatically switches to the unsteady solver, and disables all transport equation except the unsteady flamelet marker probability equation.*

(c) Click OK to close the Species Model dialog box.

2. Display the contours of probability.

   Graphics and Animations → Contours → Set Up...



   (a) Select Unsteady Flamelet... and Probability from the Contours of drop-down lists.

   (b) Ensure symmetry is selected from the Surfaces list.

   (c) Click Display (see Figure 8).

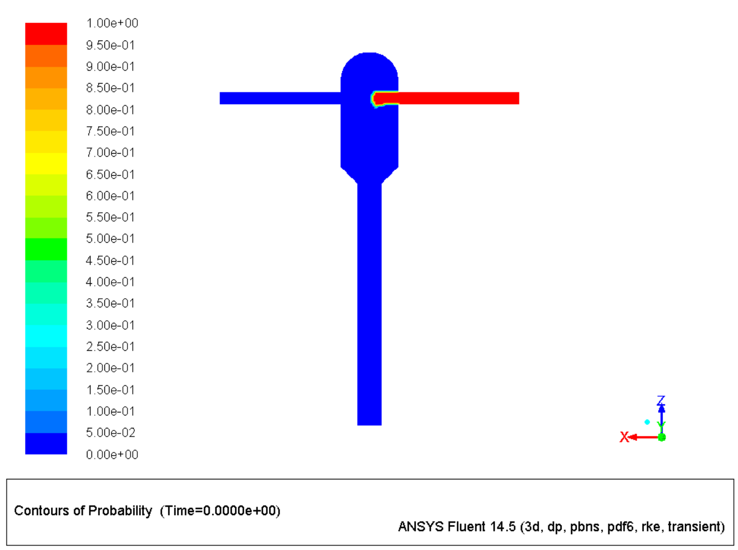


Figure 8: Contours of Probability

(d) Close the Contours dialog box.

Probability is initially set to 1 for mixture fractions greater than 0.75, and 0 everywhere else.

3. Check the solution parameters.

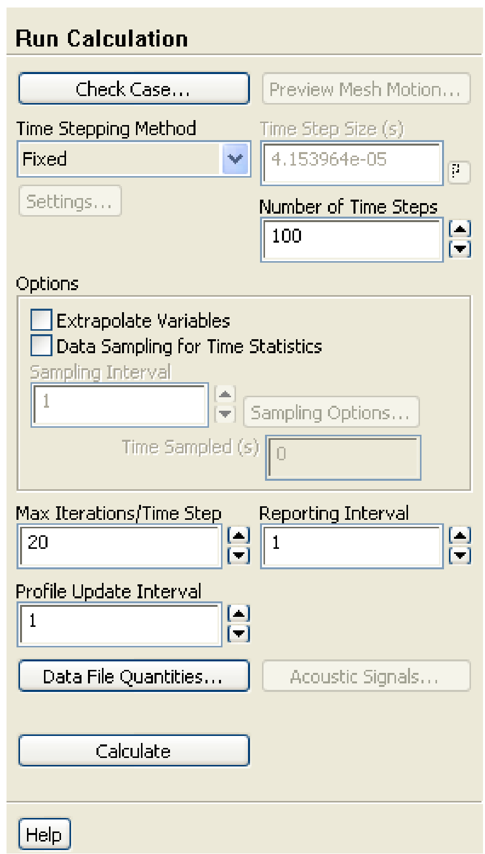
Solution Methods

(a) Ensure that Second Order Upwind is selected from the Unsteady Flamelet Probability drop-down list.

4. Save the case file (`CIJR-3.cas.gz`).

File ⟶ Write ⟶ Case...

5. Run the calculation for 100 time steps.



(a) Enter 100 for Number of Time Steps.

(b) Click Calculate.

The scaled residuals are as shown in Figure 9.

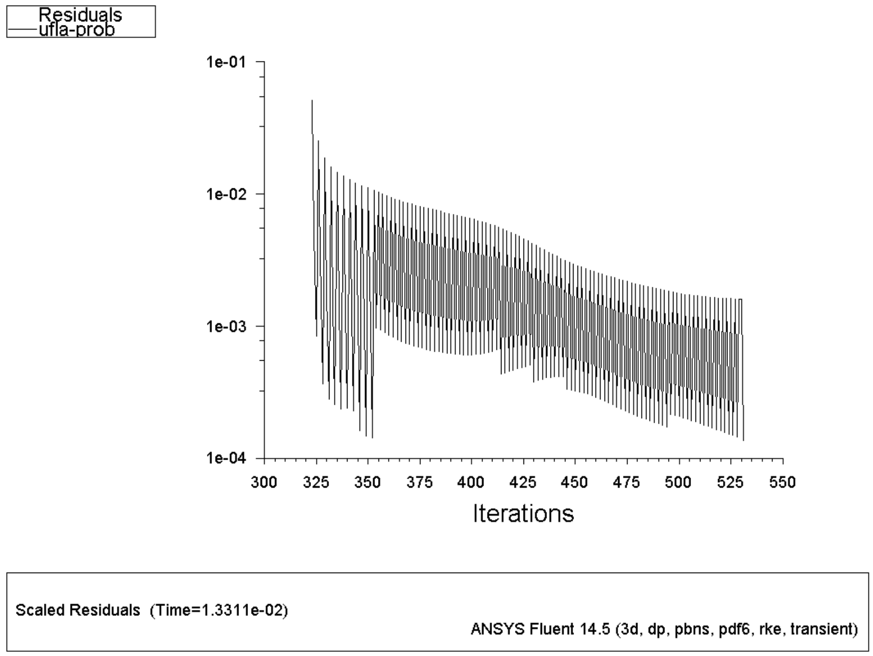


Figure 9: Scaled Residuals After Additional 100 Time Steps

The maximum probability is around 0.085 and is concentrated near the impinging jets and not near the outlet. This means that the probability marker function has not yet been fully flushed out of the domain. Hence, additional time steps are required. Instead of visually checking the probability, you could monitor the average probability at the outlet, which will initially be zero, rise in time, peak and then decrease towards zero again.

6. Save the data file (`CIJR-3.dat.gz`).

   File ⟶ Write ⟶ Data...

   The mean unsteady flamelet species converge when the probability marker has convected/diffused out of the domain. Refer to the contours of probability (see Figure 10).

7. Display the filled contours.

   Graphics and Animations ⟶ Contours ⟶ Set Up...

   (a) Select Unsteady Flamelet... and Probability from the Contours of drop-down list.

   (b) Select symmetry from the Surfaces list.

   (c) Click Display (see Figure 10).

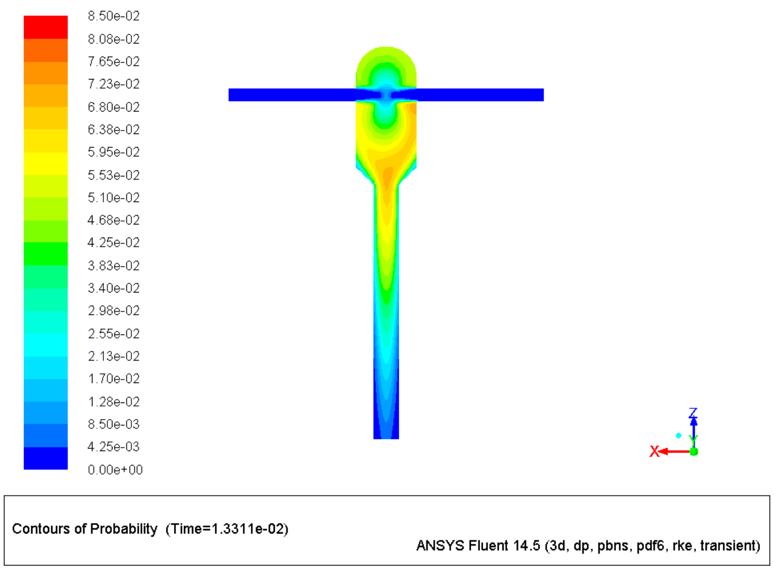


Figure 10: Contours of Probability After 100 Time Steps

(d) Close the Contours dialog box.

8. Save the case file (`CIJR-4.cas.gz`).

   File ⟶ Write ⟶ Case...

9. Run the calculation for 200 time steps.

   (a) Enter 200 for Number of Time Steps.

   (b) Click Calculate.

   The scaled residuals are as shown in Figure 11.

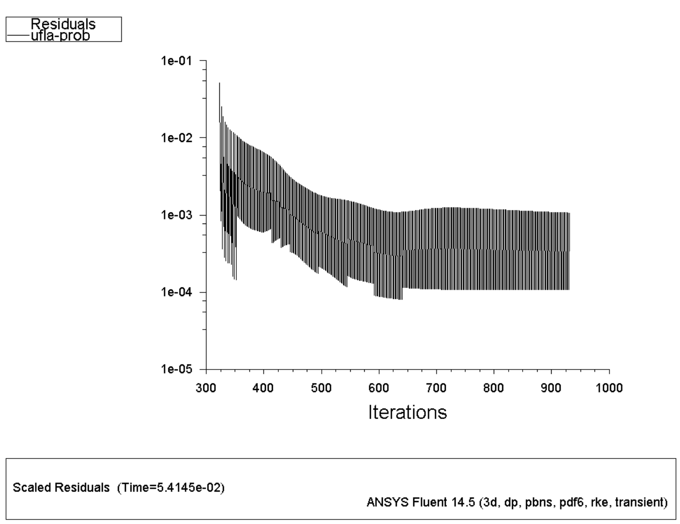


Figure 11: Scaled Residuals After Additional 200 Time Steps

10. Save the data file (`CIJR-4.dat.gz`).

    File ⟶ Write ⟶ Data...

11. Display the contours of probability.

    Graphics and Animations ⟶ Contours ⟶ Set Up...

    (a) Select Unsteady Flamelet... and Probability from the Contours of drop-down list.

    (b) Select symmetry from the Surfaces list.

    (c) Click Display (see Figure 12).

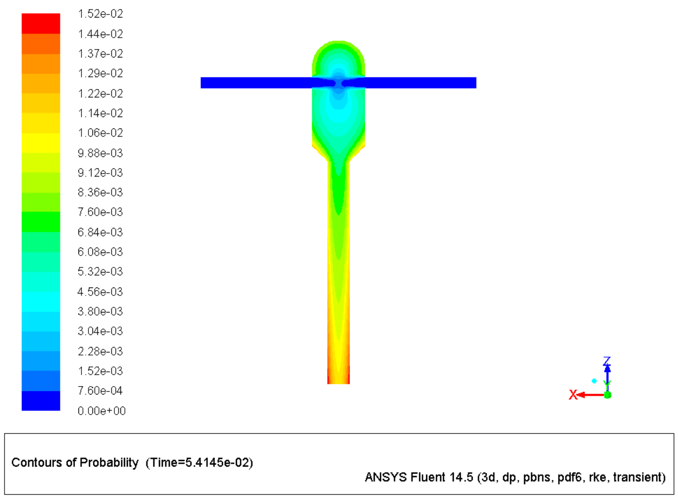


Figure 12: Contours of Probability After 200 Time Steps

    (d) Close the Contours dialog box.

The maximum probability is around 0.015 and is concentrated around the outlet. At this stage the solution can be considered to be converged and ready for postprocessing.

Step 9: Postprocessing for Unsteady Laminar Flamelet Model

1. Display the contours of mass fraction of a<l> species.

    (a) Select Unsteady Flamelet... and Mean Mass Fraction of a<l> from the Contours of drop-down list.

    (b) Click Display (see Figure 13).

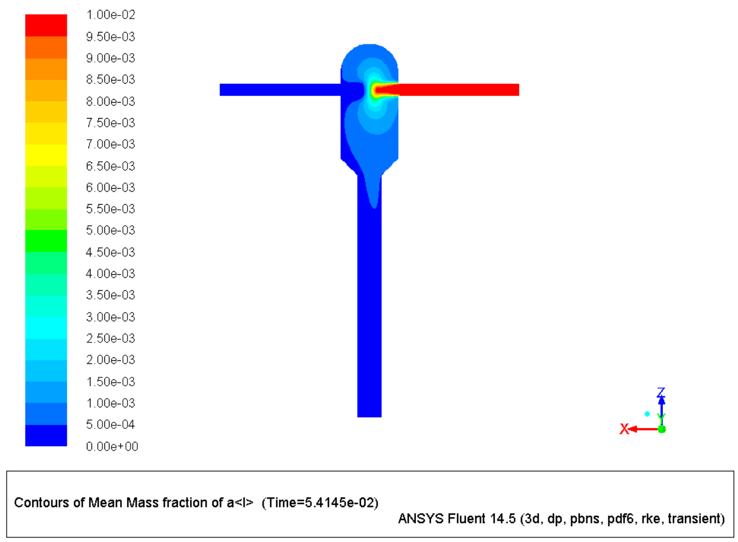


Figure 13: Contours of Mean Mass Fraction of a<l>

(c) Similarly display the contours of mass fraction of b<l> and d<l> species. Refer to Figures 14 and 15.

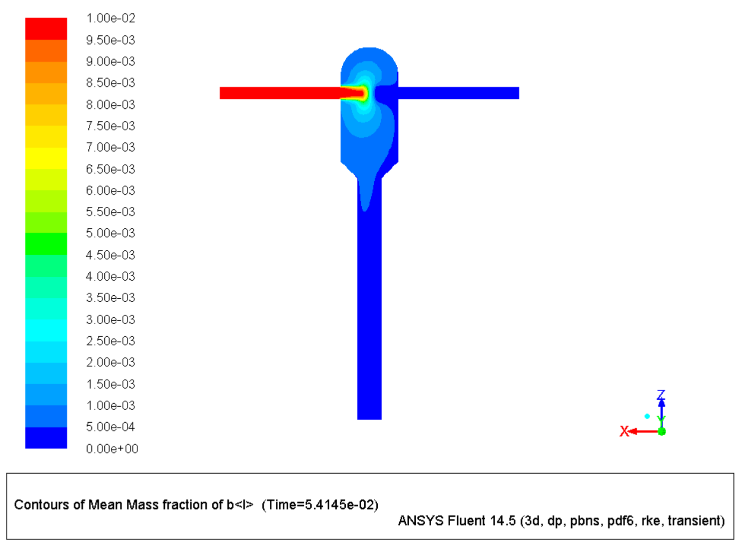


Figure 14: Contours of Mean Mass Fraction of b<l>

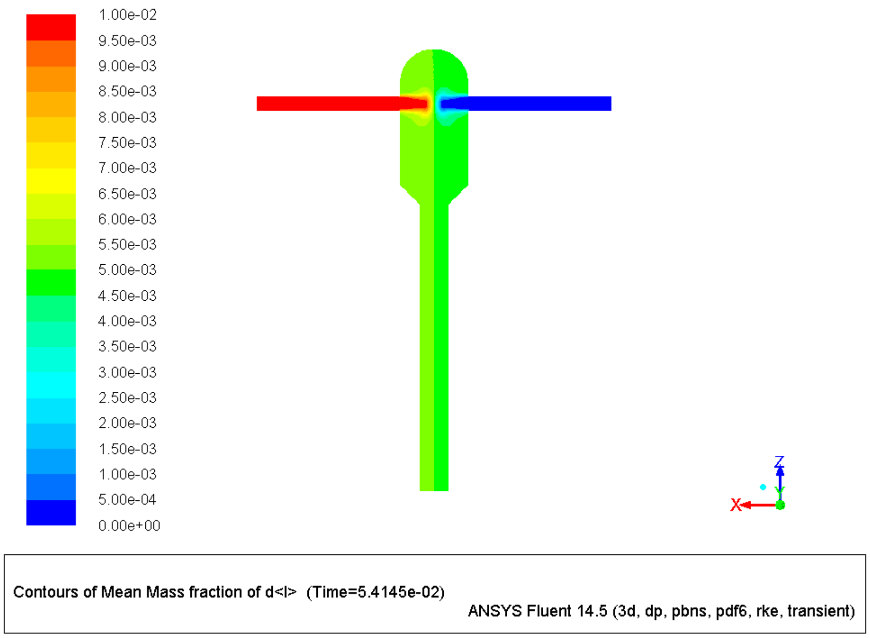


Figure 15: Contours of Mean Mass Fraction of d<l>

Since reaction 2 is much slower than reaction 1, the unsteady flamelet mass fraction of d<l> *is much different from the steady flamelet mass fraction of* d<l>.

2. Close the Contours dialog box.

Summary

This tutorial has demonstrated that the unsteady laminar flamelet model can simulate reactions in liquids with slow chemistry and low diffusivity.