Chapter 13: Modeling Species Transport and Gaseous Combustion

This tutorial is divided into the following sections:

13.1. Introduction

This tutorial examines the mixing of chemical species and the combustion of a gaseous fuel.

A cylindrical combustor burning methane (CH_4) in air is studied using the eddy-dissipation model in ANSYS Fluent.

This tutorial demonstrates how to do the following:

- Enable physical models, select material properties, and define boundary conditions for a turbulent flow with chemical species mixing and reaction.
- Initiate and solve the combustion simulation using the pressure-based solver.
- Examine the reacting flow results using graphics.
- Predict thermal and prompt NOx production.
- Use custom field functions to compute NO parts per million.

13.2. Prerequisites

This tutorial is written with the assumption that you have completed one or more of the introductory tutorials found in this manual:

- Introduction to Using ANSYS Fluent in ANSYS Workbench: Fluid Flow and Heat Transfer in a Mixing Elbow (p. 1)
- Parametric Analysis in ANSYS Workbench Using ANSYS Fluent (p. 73)
- Introduction to Using ANSYS Fluent: Fluid Flow and Heat Transfer in a Mixing Elbow (p. 121)

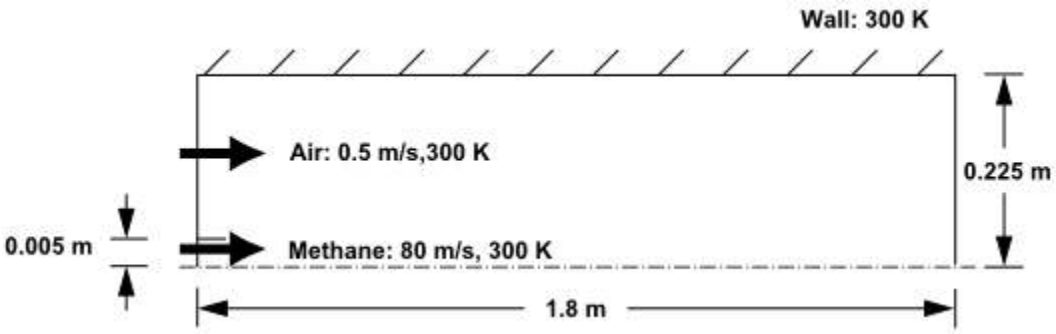
and that you are familiar with the ANSYS Fluent tree and ribbon structure. Some steps in the setup and solution procedure will not be shown explicitly.

To learn more about chemical reaction modeling, see the Fluent User's Guide and the Fluent Theory Guide. Otherwise, no previous experience with chemical reaction or combustion modeling is assumed.

13.3. Problem Description

The cylindrical combustor considered in this tutorial is shown in Figure 13.1: Combustion of Methane Gas in a Turbulent Diffusion Flame Furnace (p. 538). The flame considered is a turbulent diffusion flame. A small nozzle in the center of the combustor introduces methane at 80 m/s. Ambient air enters the combustor coaxially at 0.5 m/s. The overall equivalence ratio is approximately 0.76 (approximately 28 $\%$ excess air). The high-speed methane jet initially expands with little interference from the outer wall, and entrains and mixes with the low-speed air. The Reynolds number based on the methane jet diameter is approximately 5.7×10^3.

Figure 13.1: Combustion of Methane Gas in a Turbulent Diffusion Flame Furnace



13.4. Background

In this tutorial, you will use the generalized eddy-dissipation model to analyze the methane-air combustion system. The combustion will be modeled using a global one-step reaction mechanism, assuming complete conversion of the fuel to CO_2 and H_2O. The reaction equation is

$$CH_4+2O_2\rightarrow CO_2+2H_2O \tag{13.1}$$

This reaction will be defined in terms of stoichiometric coefficients, formation enthalpies, and parameters that control the reaction rate. The reaction rate will be determined assuming that turbulent mixing is the rate-limiting process, with the turbulence-chemistry interaction modeled using the eddy-dissipation model.

13.5. Setup and Solution

The following sections describe the setup and solution steps for this tutorial:

13.5.1. Preparation

To prepare for running this tutorial:

1. Set up a working folder on the computer you will be using.
2. Go to the ANSYS Customer Portal, https://support.ansys.com/training.

   Note

   If you do not have a login, you can request one by clicking **Customer Registration** on the log in page.

3. Enter the name of this tutorial into the search bar.
4. Narrow the results by using the filter on the left side of the page.
   a. Click **ANSYS Fluent** under **Product**.
   b. Click **18.0** under **Version**.
5. Select this tutorial from the list.
6. Click the **species_transport_R180.zip** link to download the input files.
7. Unzip `species_transport_R180.zip` to your working folder.

   The file `gascomb.msh` can be found in the `species_transport` folder created after unzipping the file.
8. Use Fluent Launcher to start the **2D** version of ANSYS Fluent.

   Fluent Launcher displays your **Display Options** preferences from the previous session.

   For more information about Fluent Launcher, see starting ANSYS Fluent using the Fluent Launcher in the Fluent Getting Started Guide.
9. Ensure that the **Display Mesh After Reading** and **Workbench Color Scheme** options are enabled.
10. Enable **Double-Precision**.
11. Ensure **Serial** is selected under **Processing Options**.

13.5.2. Mesh

1. Read the mesh file `gascomb.msh`.

   File → Read → Mesh...

   After reading the mesh file, ANSYS Fluent will report that 1615 quadrilateral fluid cells have been read, along with a number of boundary faces with different zone identifiers.

13.5.3. General Settings

1. Check the mesh.

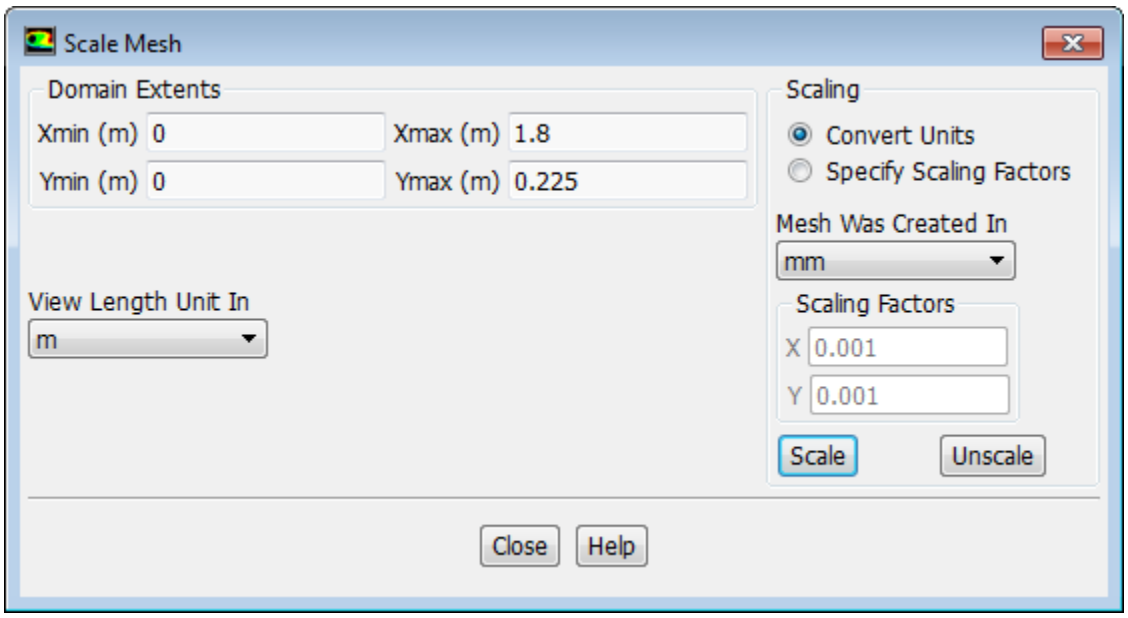
Setting Up Domain → Mesh → Check

ANSYS Fluent will perform various checks on the mesh and will report the progress in the console. Ensure that the reported minimum volume reported is a positive number.

2. Scale the mesh.

Setting Up Domain → Mesh → Scale...

Since this mesh was created in units of millimeters, you will need to scale the mesh into meters.



a. Select **mm** from the **Mesh Was Created In** drop-down list in the **Scaling** group box.

b. Click **Scale**.

c. Ensure that **m** is selected from the **View Length Unit In** drop-down list.

d. Ensure that **Xmax** and **Ymax** are reset to 1.8 m and 0.225 m respectively.

The default SI units will be used in this tutorial, hence there is no need to change any units in this problem.

e. Close the **Scale Mesh** dialog box.

3. Check the mesh.

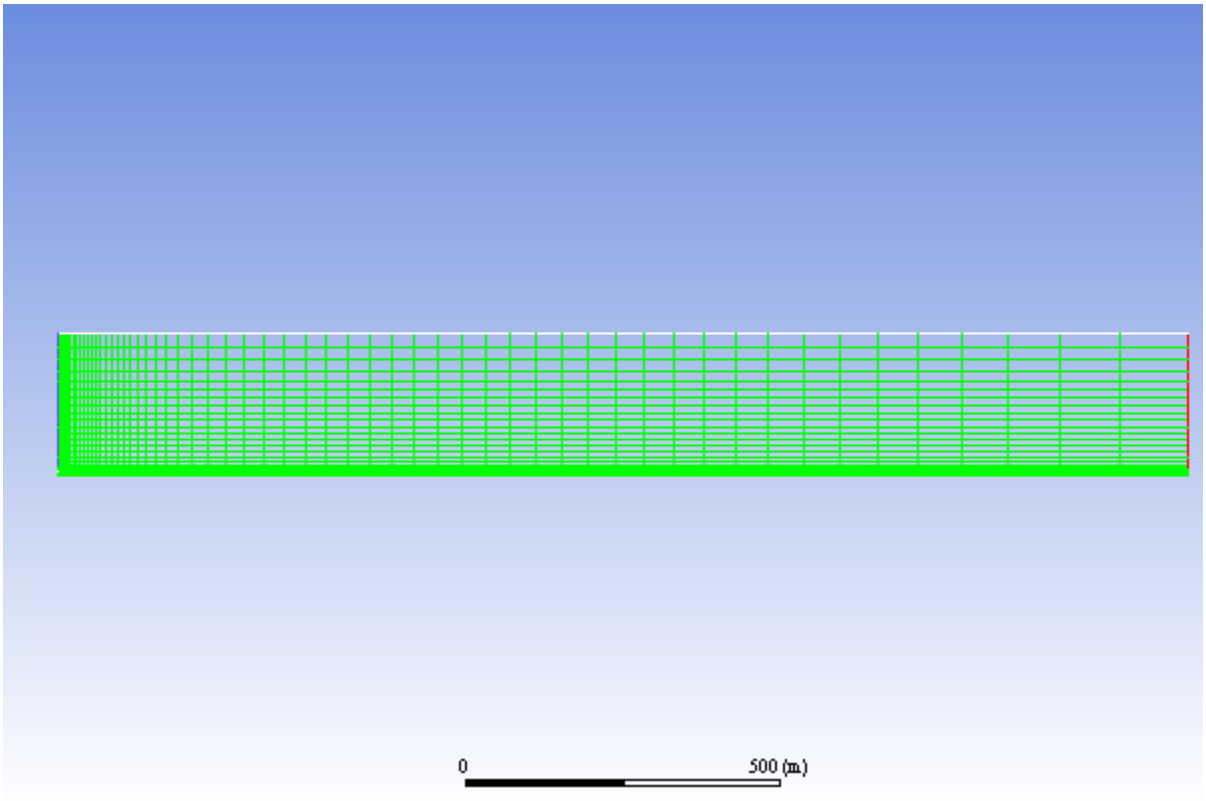
Setting Up Domain → Mesh → Check

Note

You should check the mesh after you manipulate it (scale, convert to polyhedra, merge, separate, fuse, add zones, or smooth and swap). This will ensure that the quality of the mesh has not been compromised.

4. Examine the mesh with the default settings.

Figure 13.2: The Quadrilateral Mesh for the Combustor Model

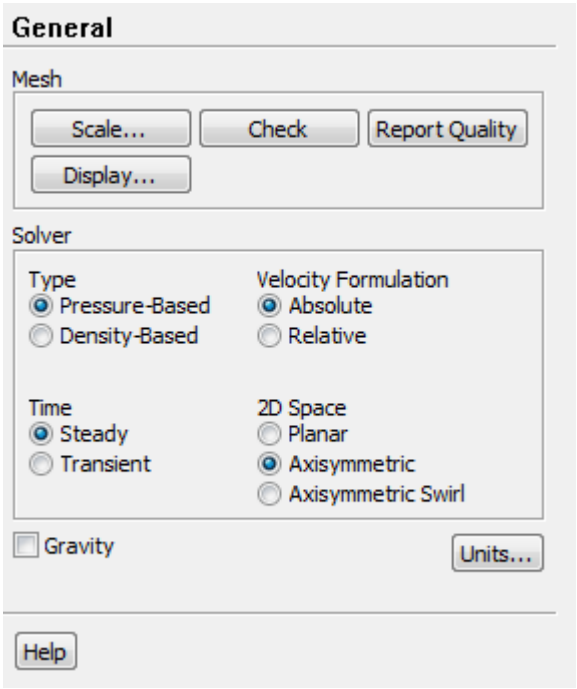


Extra

You can use the right mouse button to probe for mesh information in the graphics window. If you click the right mouse button on any node in the mesh, information will be displayed in the ANSYS Fluent console about the associated zone, including the name of the zone. This feature is especially useful when you have several zones of the same type and you want to distinguish between them quickly.

5. Select **Axisymmetric** in the **2D Space** list.

Setup → General



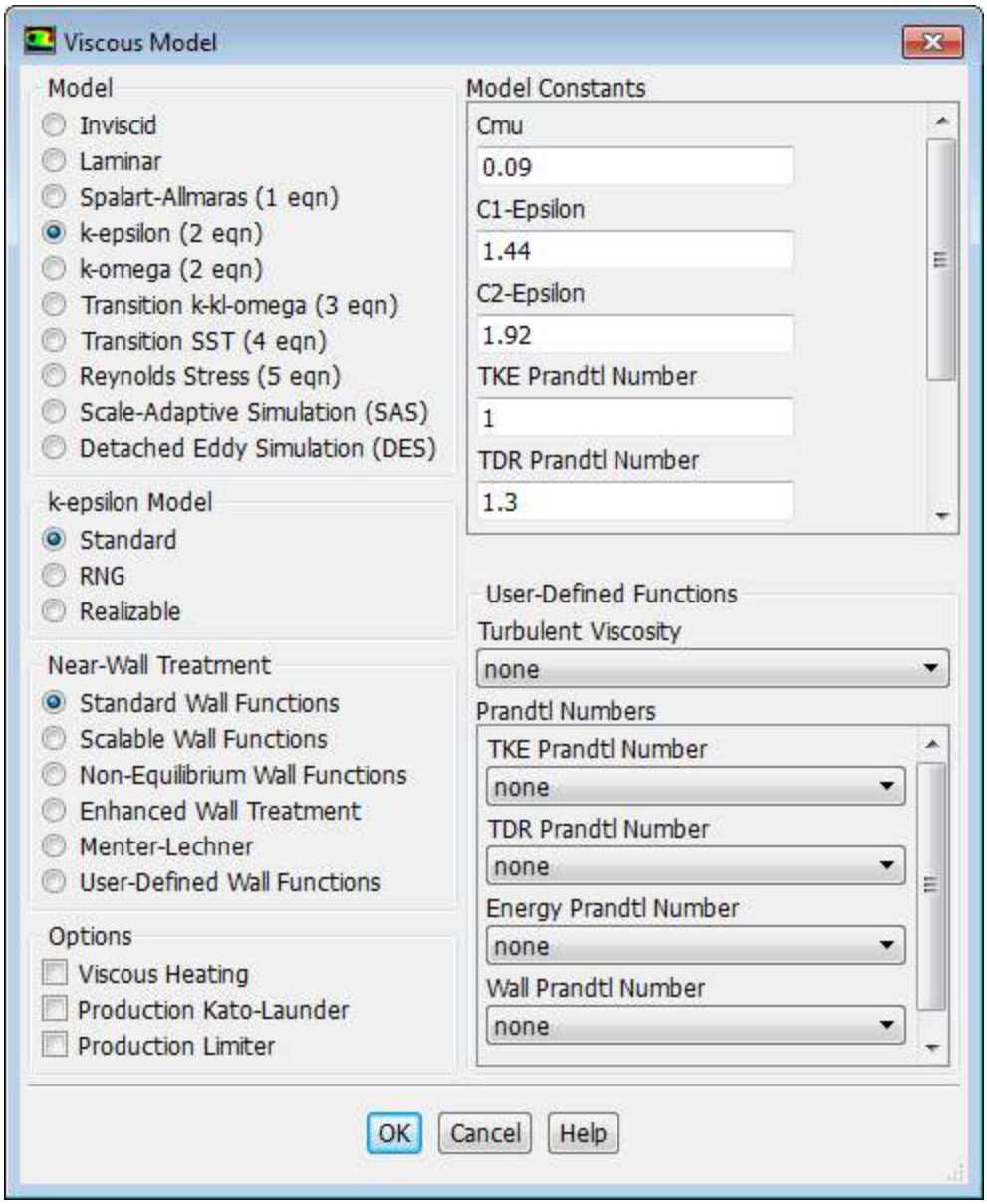
13.5.4. Models

1. Enable heat transfer by enabling the energy equation.

   Setting Up Physics → Models → Energy

2. Select the standard k-ε turbulence model.

   Setting Up Physics → Models → Viscous...



a. Select **k-epsilon (2 eqn)** in the **Model** list.

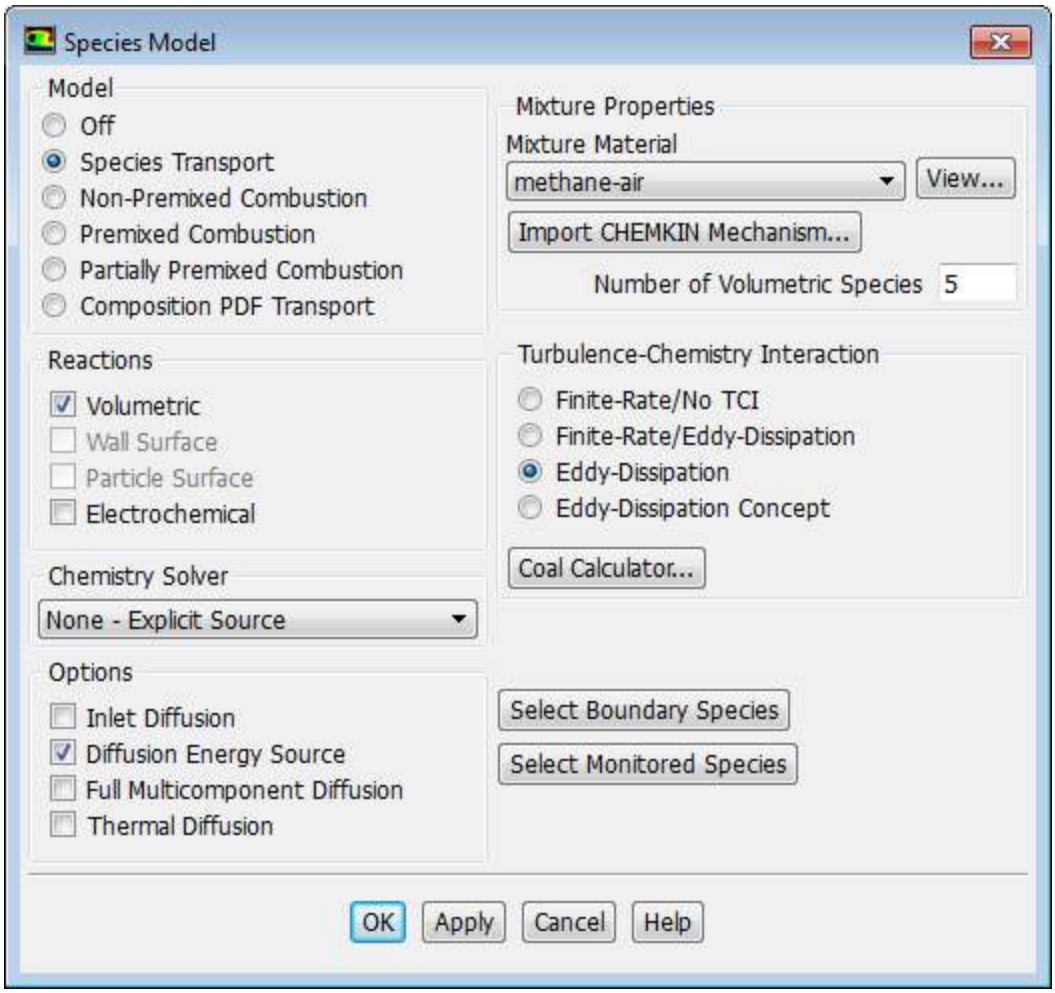
   *The **Viscous Model** dialog box will expand to provide further options for the **k-epsilon** model.*

b. Retain the default settings for the **k-epsilon** model.

c. Click **OK** to close the **Viscous Model** dialog box.

3. Enable chemical species transport and reaction.

   Setting Up Physics → Models → Species...



a. Select **Species Transport** in the **Model** list.

   *The **Species Model** dialog box will expand to provide further options for the **Species Transport** model.*

b. Enable **Volumetric** in the **Reactions** group box.

c. Select **methane-air** from the **Mixture Material** drop-down list.

   *Scroll down the list to find **methane-air**.*

   Note

   The **Mixture Material** list contains the set of chemical mixtures that exist in the ANSYS Fluent database. You can select one of the predefined mixtures to access a complete description of the reacting system. The chemical species in the system and their physical and thermodynamic properties are defined by your selection of the mixture material. You can alter the mixture material selection or modify the mixture material properties using the **Create/Edit Materials** dialog box (see Materials (p. 545)).

d. Select **Eddy-Dissipation** in the **Turbulence-Chemistry Interaction** group box.

The eddy-dissipation model computes the rate of reaction under the assumption that chemical kinetics are fast compared to the rate at which reactants are mixed by turbulent fluctuations (eddies).

e. Click **OK** to close the **Species Model** dialog box.

Prior to listing the properties that are required for the models you have enabled, ANSYS Fluent will display a warning about the symmetry zone in the console. You may have to scroll up to see this warning.

```
Warning: It appears that symmetry zone 5 should actually be an axis
         (it has faces with zero area projections).
         Unless you change the zone type from symmetry to axis,
         you may not be able to continue the solution without
         encountering floating point errors.
```

In the axisymmetric model, the boundary conditions should be such that the centerline is an axis type instead of a symmetry type. You will change the symmetry zone to an axis boundary in *Boundary Conditions (p. 548)**.*

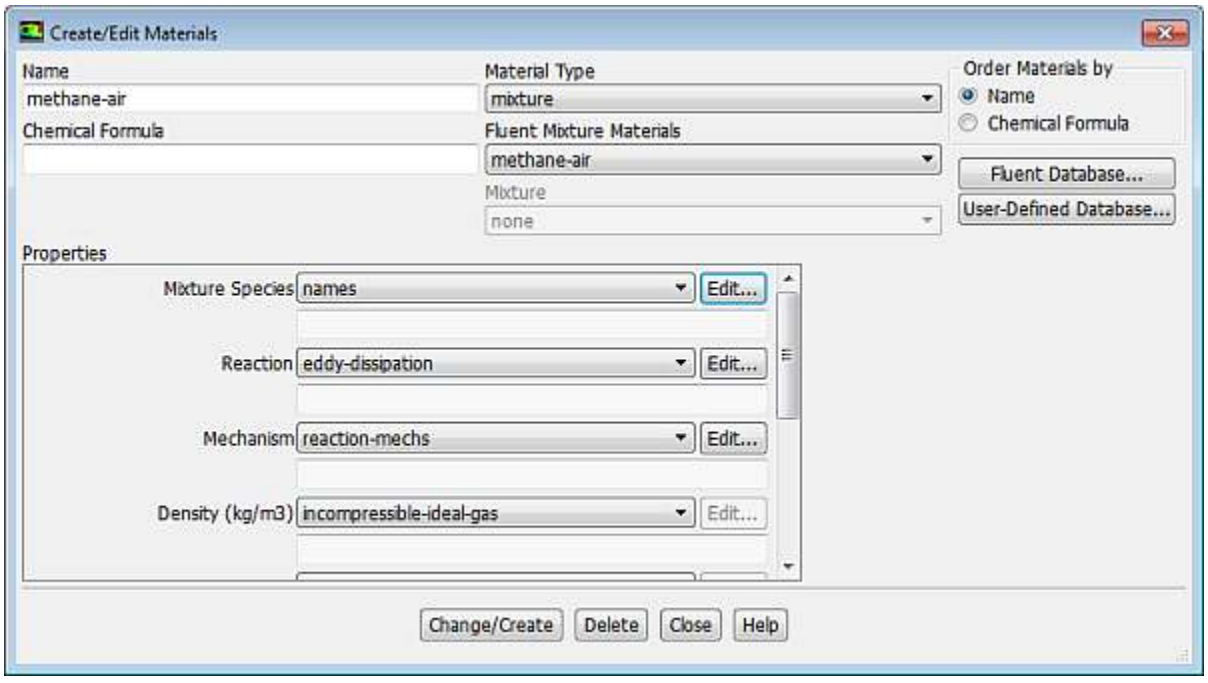
13.5.5. Materials

In this step, you will examine the default settings for the mixture material. This tutorial uses mixture properties copied from the Fluent Database. In general, you can modify these or create your own mixture properties for your specific problem as necessary.

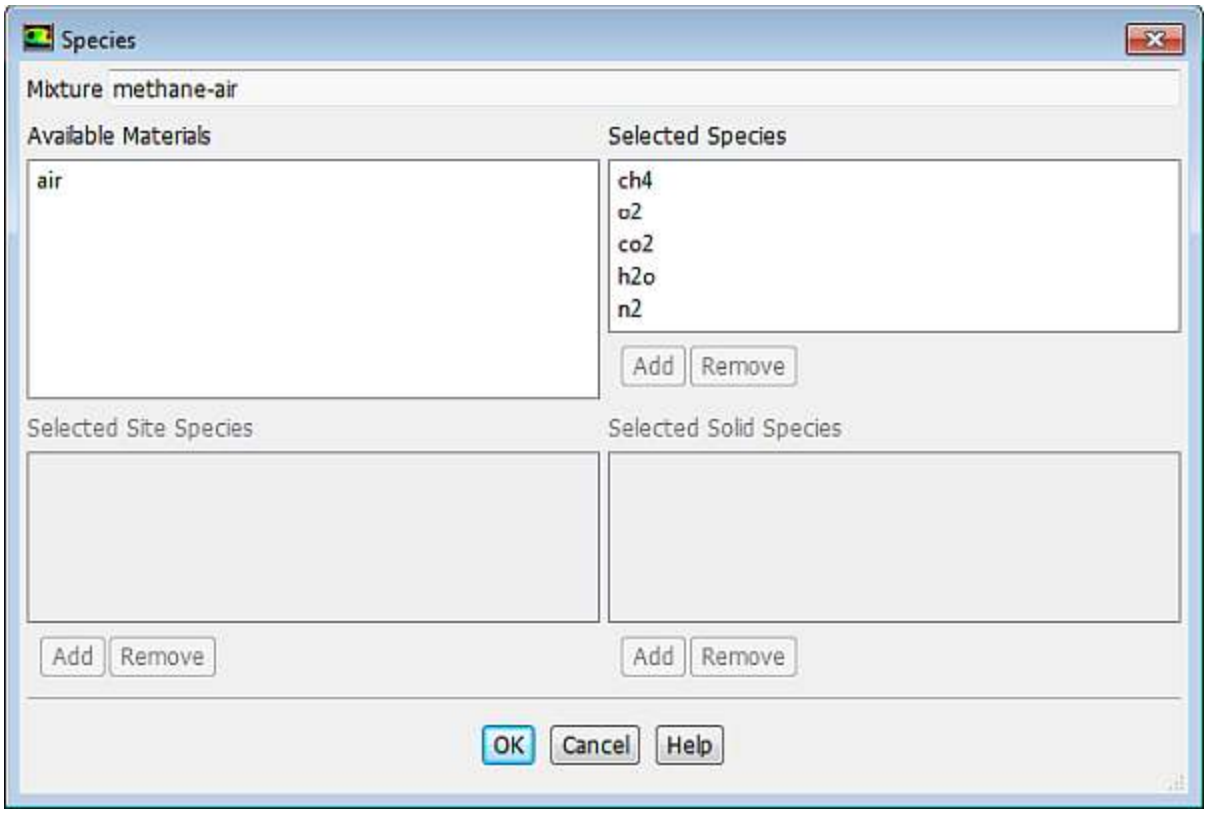
1. Confirm the properties for the mixture materials.

Setup → Materials → Mixture → methane-air Edit...

*The **Create/Edit Materials** dialog box will display the mixture material (**methane-air**) that was selected in the **Species Model** dialog box. The properties for this mixture material have been copied from the **Fluent Database...** and will be modified in the following steps.*



a. Click the **Edit...** button to the right of the **Mixture Species** drop-down list to open the **Species** dialog box.



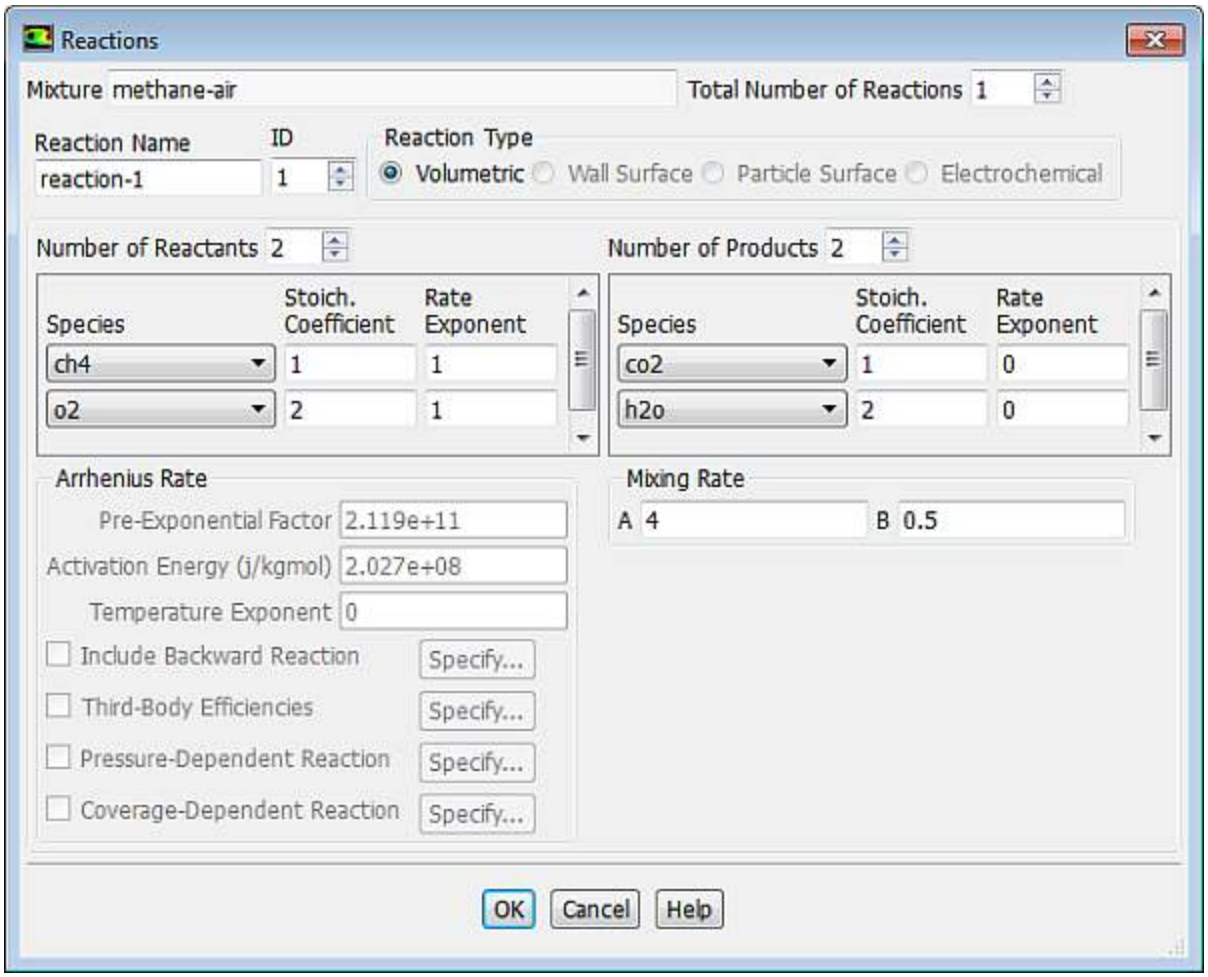
*You can add or remove species from the mixture material as necessary using the **Species** dialog box.*

i. Retain the default selections from the **Selected Species** selection list.

The species that make up the methane-air mixture are predefined and require no modification.

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

b. Click the **Edit...** button to the right of the **Reaction** drop-down list to open the **Reactions** dialog box.



*The eddy-dissipation reaction model ignores chemical kinetics (the Arrhenius rate) and uses only the parameters in the **Mixing Rate** group box in the **Reactions** dialog box. The **Arrhenius Rate** group box will therefore be inactive. The values for **Rate Exponent** and **Arrhenius Rate** parameters are included in the database and are employed when the alternate finite-rate/eddy-dissipation model is used.*

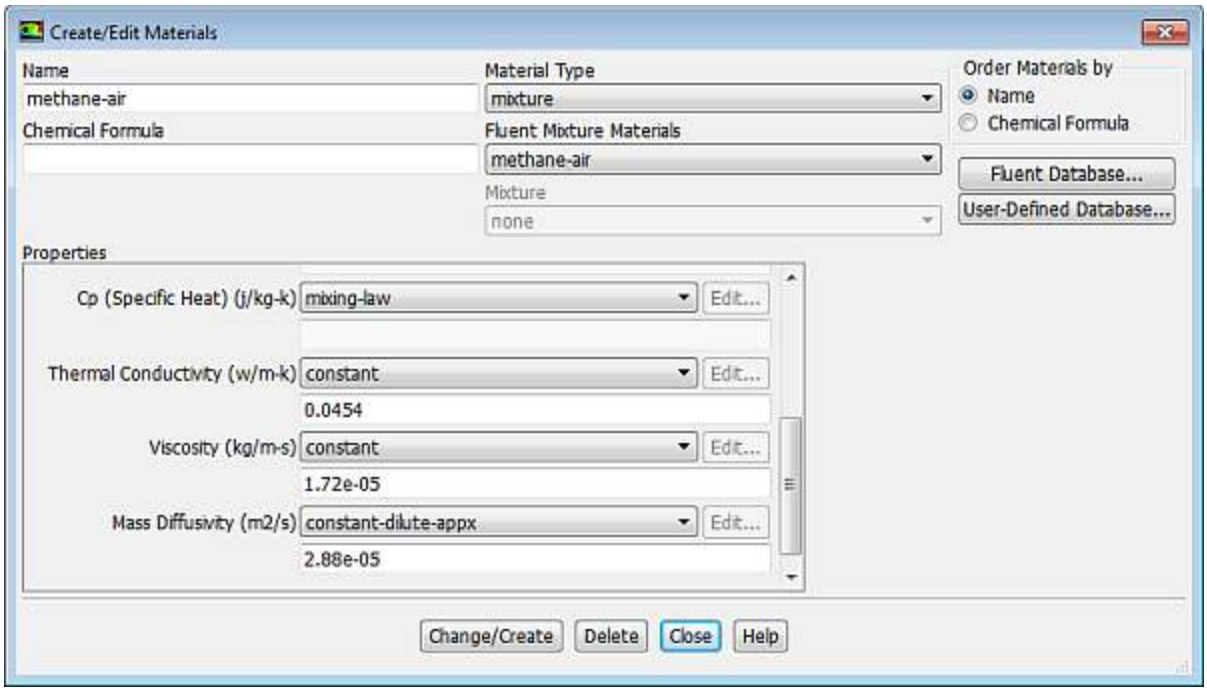
i. Retain the default values in the **Mixing Rate** group box.

ii. Click **OK** to close the **Reactions** dialog box.

c. Retain the selection of **incompressible-ideal-gas** from the **Density** drop-down list.

d. Retain the selection of **mixing-law** from the **Cp (Specific Heat)** drop-down list.

e. Retain the default values for **Thermal Conductivity**, **Viscosity**, and **Mass Diffusivity**.



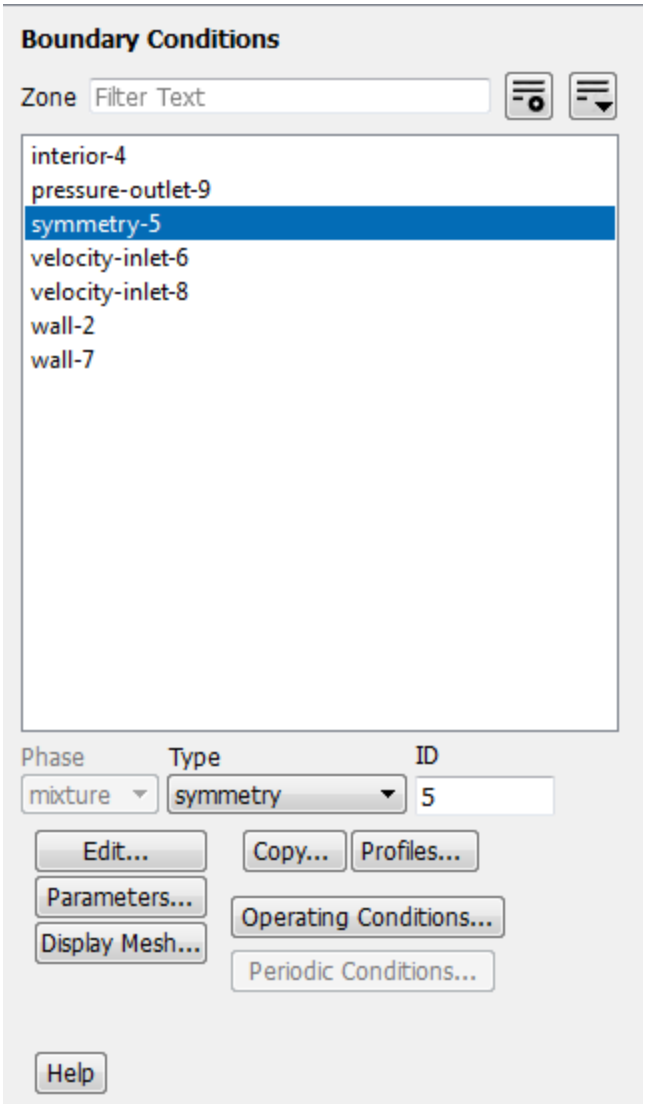
f. Click **Change/Create** to accept the material property settings.

g. Close the **Create/Edit Materials** dialog box.

The calculation will be performed assuming that all properties except density and specific heat are constant. The use of constant transport properties (viscosity, thermal conductivity, and mass diffusivity coefficients) is acceptable because the flow is fully turbulent. The molecular transport properties will play a minor role compared to turbulent transport.

13.5.6. Boundary Conditions

Setup → Boundary Conditions



1. Convert the symmetry zone to the axis type.

   Setup → **Boundary Conditions** → **symmetry-5**

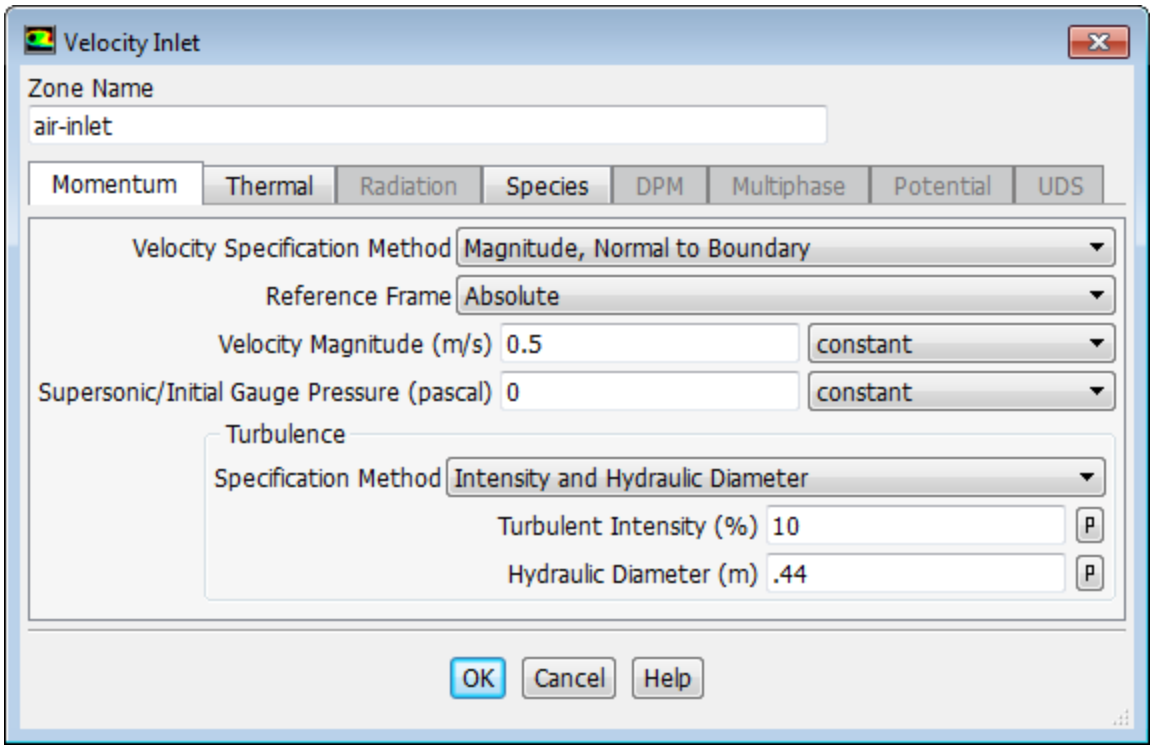
   The symmetry zone must be converted to an axis to prevent numerical difficulties where the radius reduces to zero.

   a. Select **axis** from the **Type** drop-down list.

2. Set the boundary conditions for the air inlet (**velocity-inlet-8**).

   Setup → **Boundary Conditions** → **velocity-inlet-8** **Edit...**

   *To determine the zone for the air inlet, display the mesh without the fluid zone to see the boundaries. Use the right mouse button to probe the air inlet. ANSYS Fluent will report the zone name (**velocity-inlet-8**) in the console.*



a. Enter `air-inlet` for **Zone Name**.

   *This name is more descriptive for the zone than **velocity-inlet-8**.*

b. Enter `0.5` m/s for **Velocity Magnitude**.

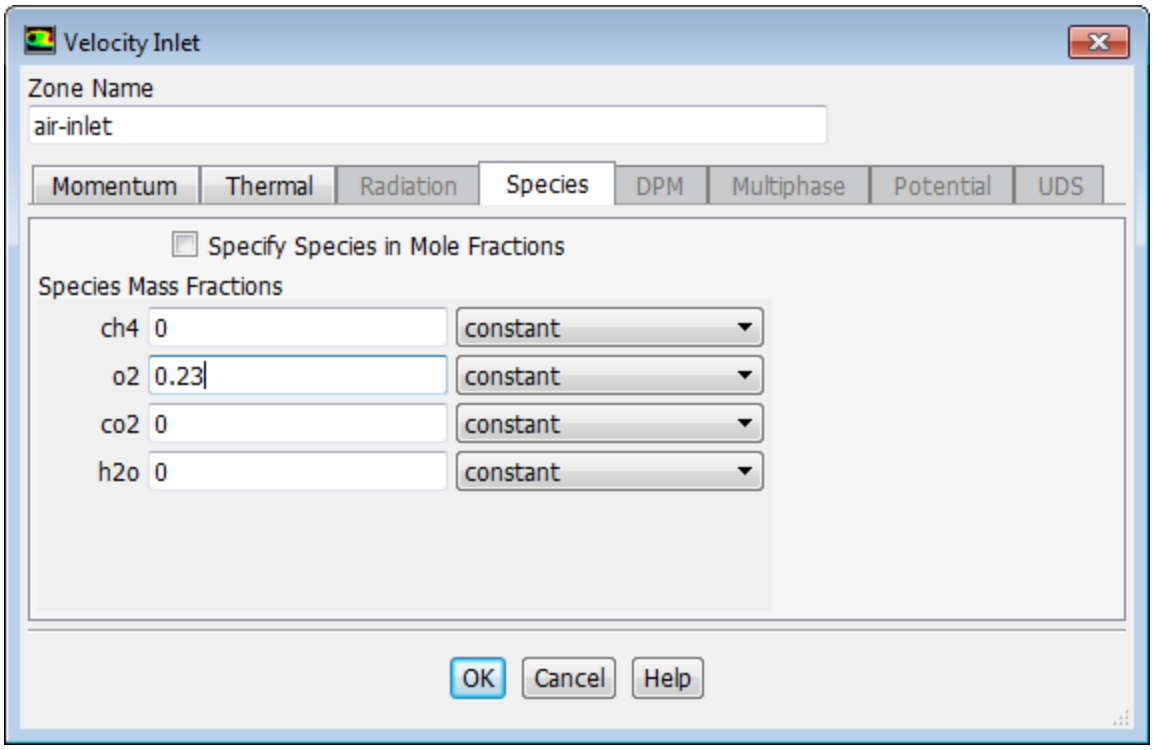
c. Select **Intensity and Hydraulic Diameter** from the **Specification Method** drop-down list in the **Turbulence** group box.

d. Enter `10` $\%$ for **Turbulent Intensity**.

e. Enter `0.44` m for **Hydraulic Diameter**.

f. Click the **Thermal** tab and retain the default value of `300` K for **Temperature**.

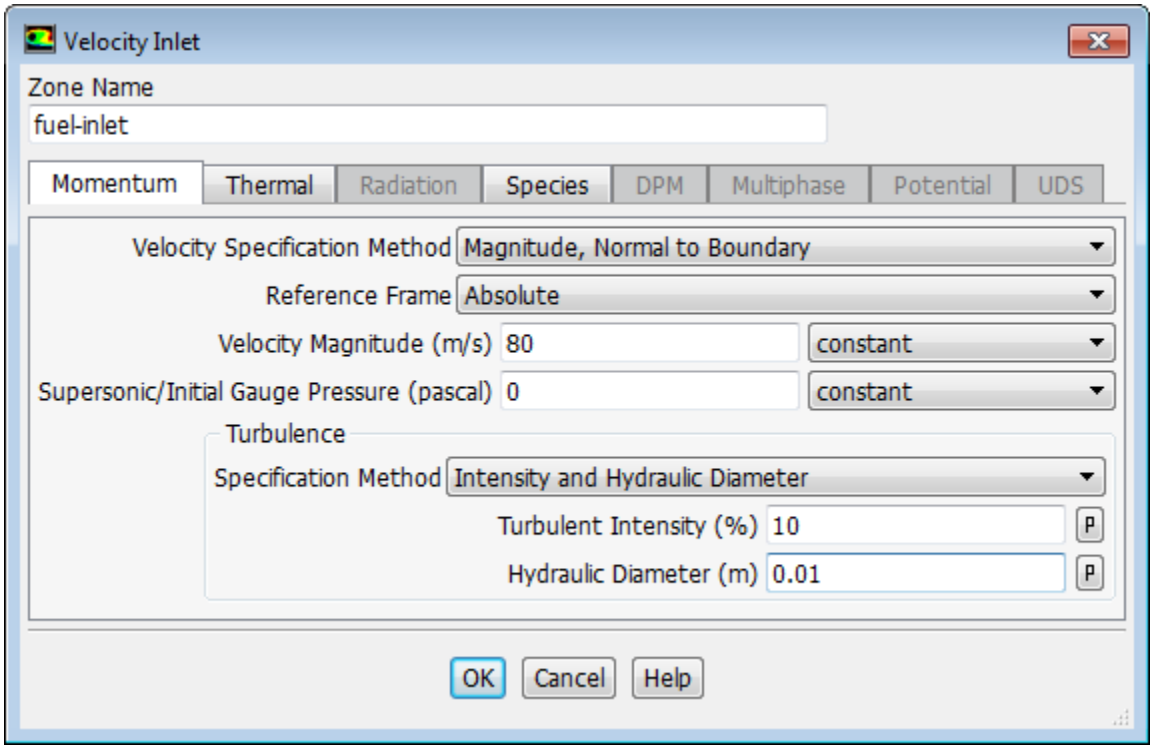
g. Click the **Species** tab and enter `0.23` for **o2** in the **Species Mass Fractions** group box.



h. Click **OK** to close the **Velocity Inlet** dialog box.

3. Set the boundary conditions for the fuel inlet (**velocity-inlet-6**).

Setup → **Boundary Conditions** → **velocity-inlet-6** **Edit...**



a. Enter `fuel-inlet` for **Zone Name**.

This name is more descriptive for the zone than ***velocity-inlet-6****.*

b. Enter `80` m/s for the **Velocity Magnitude**.

c. Select **Intensity and Hydraulic Diameter** from the **Specification Method** drop-down list in the **Turbulence** group box.

d. Enter `10` $\%$ for **Turbulent Intensity**.

e. Enter `0.01` m for **Hydraulic Diameter**.

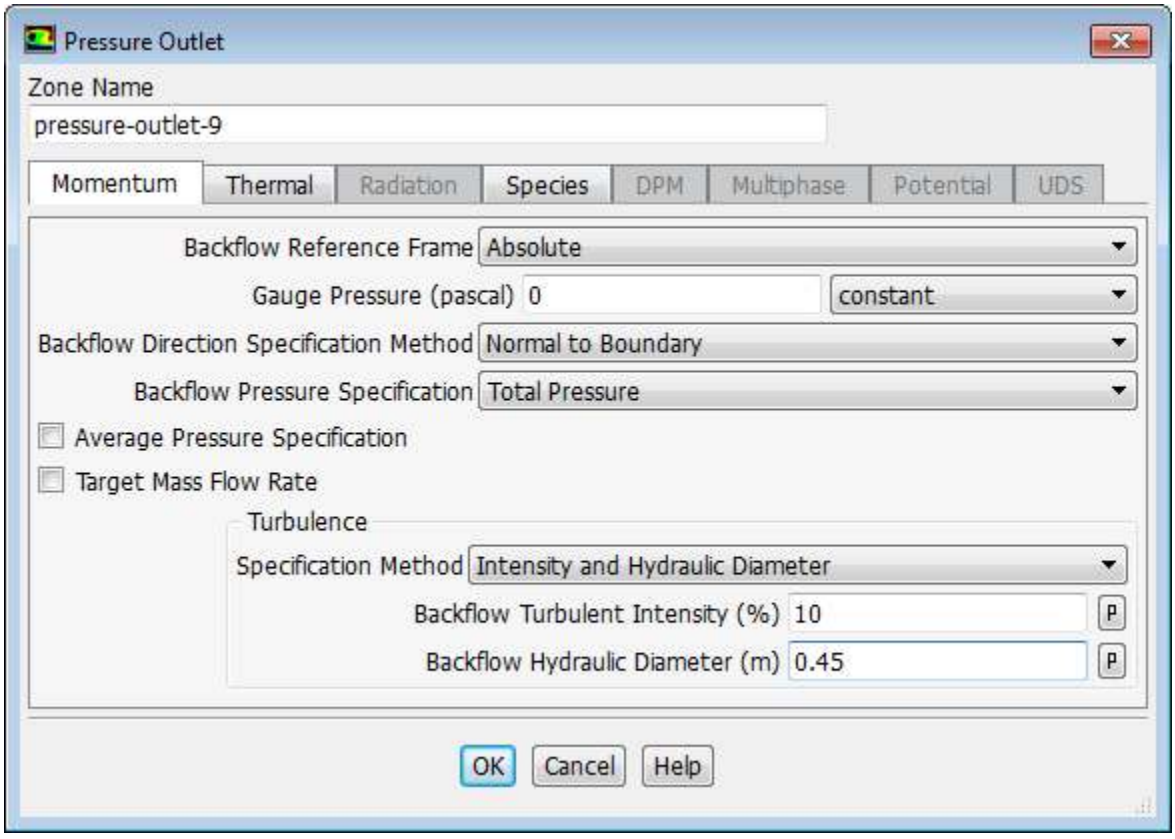
f. Click the **Thermal** tab and retain the default value of `300` K for **Temperature**.

g. Click the **Species** tab and enter `1` for **ch4** in the **Species Mass Fractions** group box.

h. Click **OK** to close the **Velocity Inlet** dialog box.

4. Set the boundary conditions for the exit boundary (**pressure-outlet-9**).

Setup → Boundary Conditions → pressure-outlet-9 Edit...



a. Retain the default value of `0` Pa for **Gauge Pressure**.

b. Select **Intensity and Hydraulic Diameter** from the **Specification Method** drop-down list in the **Turbulence** group box.

c. Enter `10` $\%$ for **Backflow Turbulent Intensity**.

d. Enter `0.45` m for **Backflow Hydraulic Diameter**.

e. Click the **Thermal** tab and retain the default value of `300` K for **Backflow Total Temperature**.

f. Click the **Species** tab and enter `0.23` for **o2** in the **Species Mass Fractions** group box.

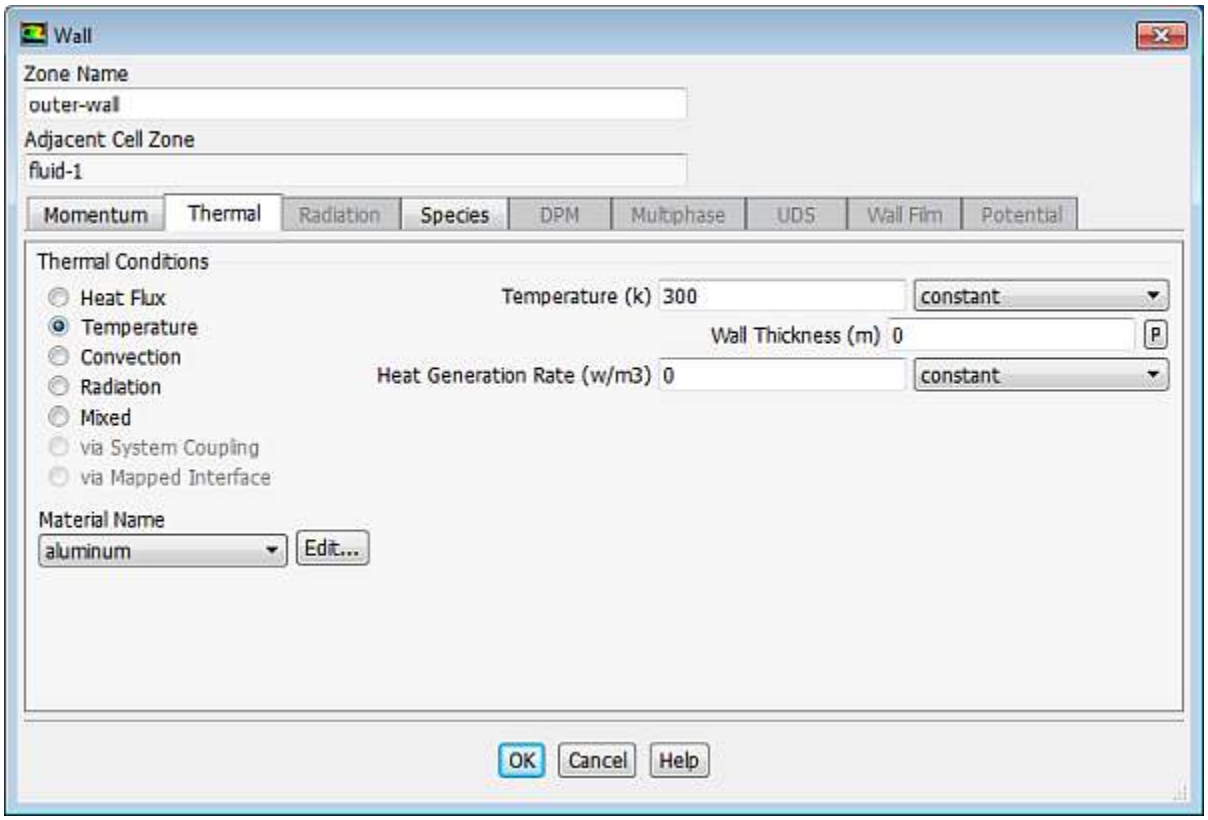
g. Click **OK** to close the **Pressure Outlet** dialog box.

*The **Backflow** values in the **Pressure Outlet** dialog box are utilized only when backflow occurs at the pressure outlet. Always assign reasonable values because backflow may occur during intermediate iterations and could affect the solution stability.*

5. Set the boundary conditions for the outer wall (**wall-7**).

Setup → Boundary Conditions → wall-7 Edit...

Use the mouse-probe method described for the air inlet to determine the zone corresponding to the outer wall.



a. Enter `outer-wall` for **Zone Name**.

*This name is more descriptive for the zone than **wall-7**.*

b. Click the **Thermal** tab.

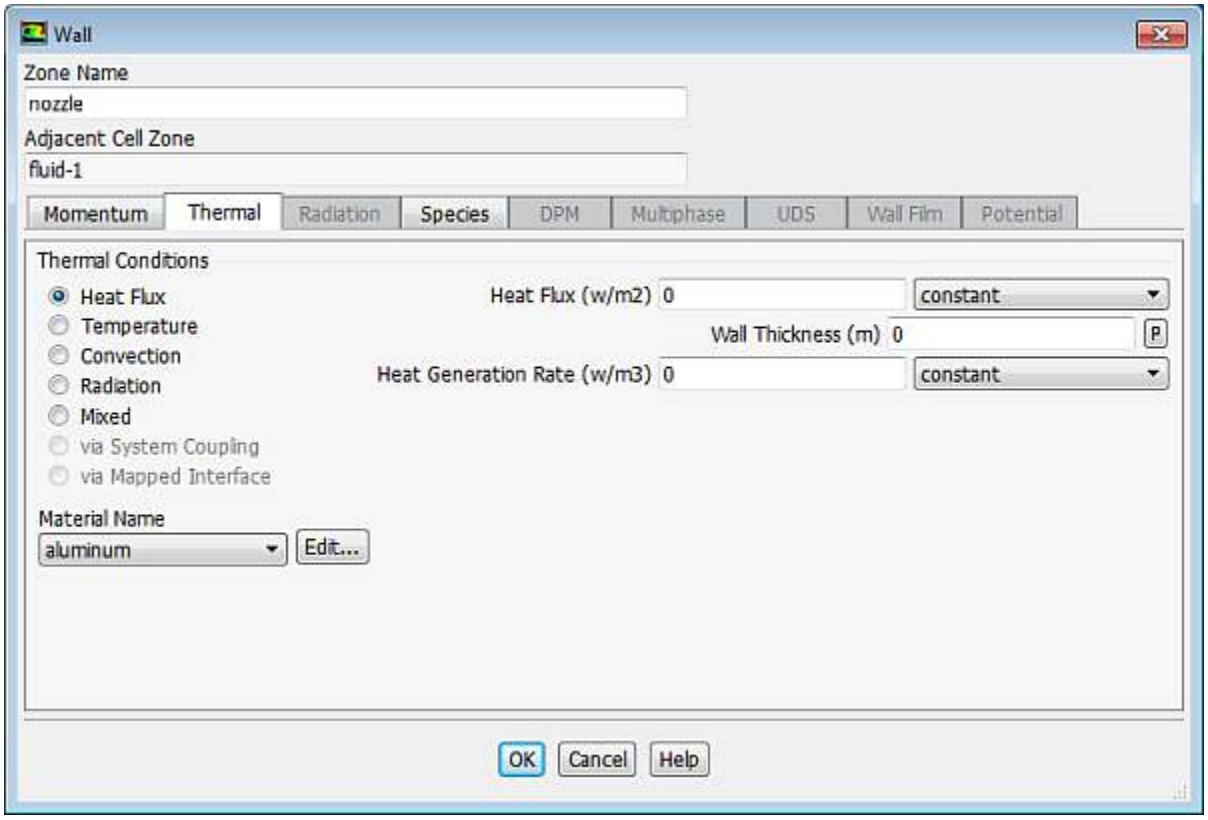
i. Select **Temperature** in the **Thermal Conditions** list.

ii. Retain the default value of `300` K for **Temperature**.

c. Click **OK** to close the **Wall** dialog box.

6. Set the boundary conditions for the fuel inlet nozzle (**wall-2**).

   Setup → **Boundary Conditions** → **wall-2** **Edit...**



   a. Enter `nozzle` for **Zone Name**.

      *This name is more descriptive for the zone than **wall-2**.*

   b. Click the **Thermal** tab.

      i. Retain the default selection of **Heat Flux** in the **Thermal Conditions** list.

      ii. Retain the default value of `0` W / m^2 for **Heat Flux**, so that the wall is adiabatic.

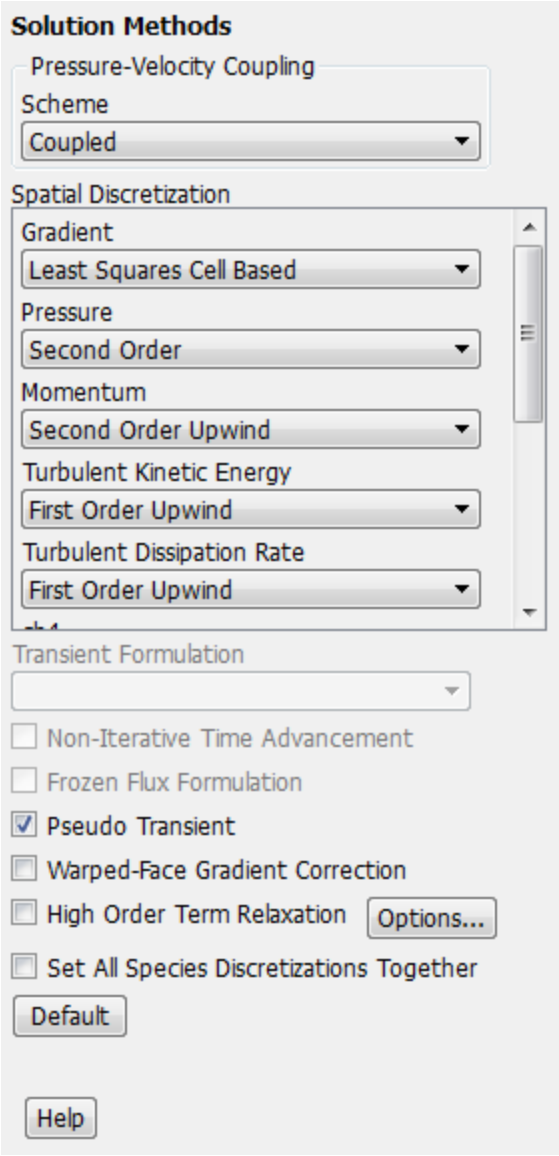
   c. Click **OK** to close the **Wall** dialog box.

13.5.7. Initial Reaction Solution

You will first calculate a solution for the basic reacting flow neglecting pollutant formation. In a later step, you will perform an additional analysis to simulate NOx.

1. Select the Coupled Pseudo Transient solution method.

   Solving → **Solution** → **Methods...**



a. Select **Coupled** from the **Scheme** drop-down list in the **Pressure-Velocity Coupling** group box.

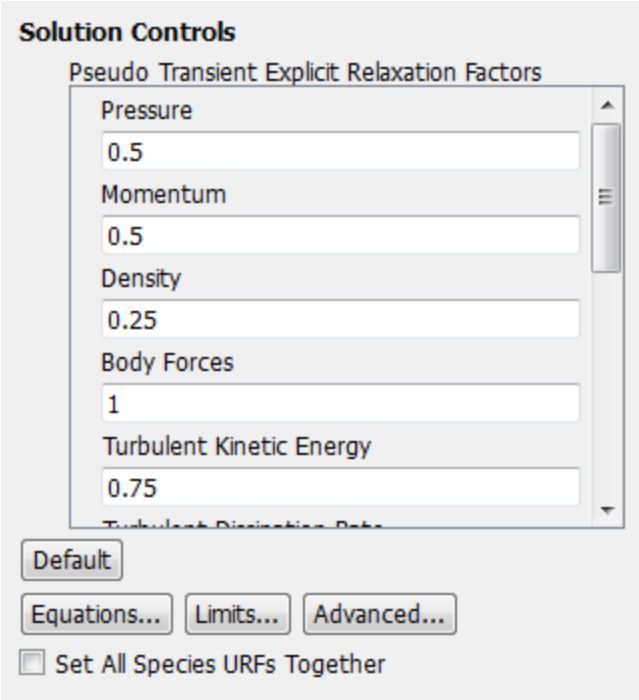
b. Retain the default selections in the **Spatial Discretization** group box.

c. Enable **Pseudo Transient**.

The Pseudo Transient option enables the pseudo transient algorithm in the coupled pressure-based solver. This algorithm effectively adds an unsteady term to the solution equations in order to improve stability and convergence behavior. Use of this option is recommended for general fluid flow problems.

2. Modify the solution controls.

Solving → Controls → Controls...

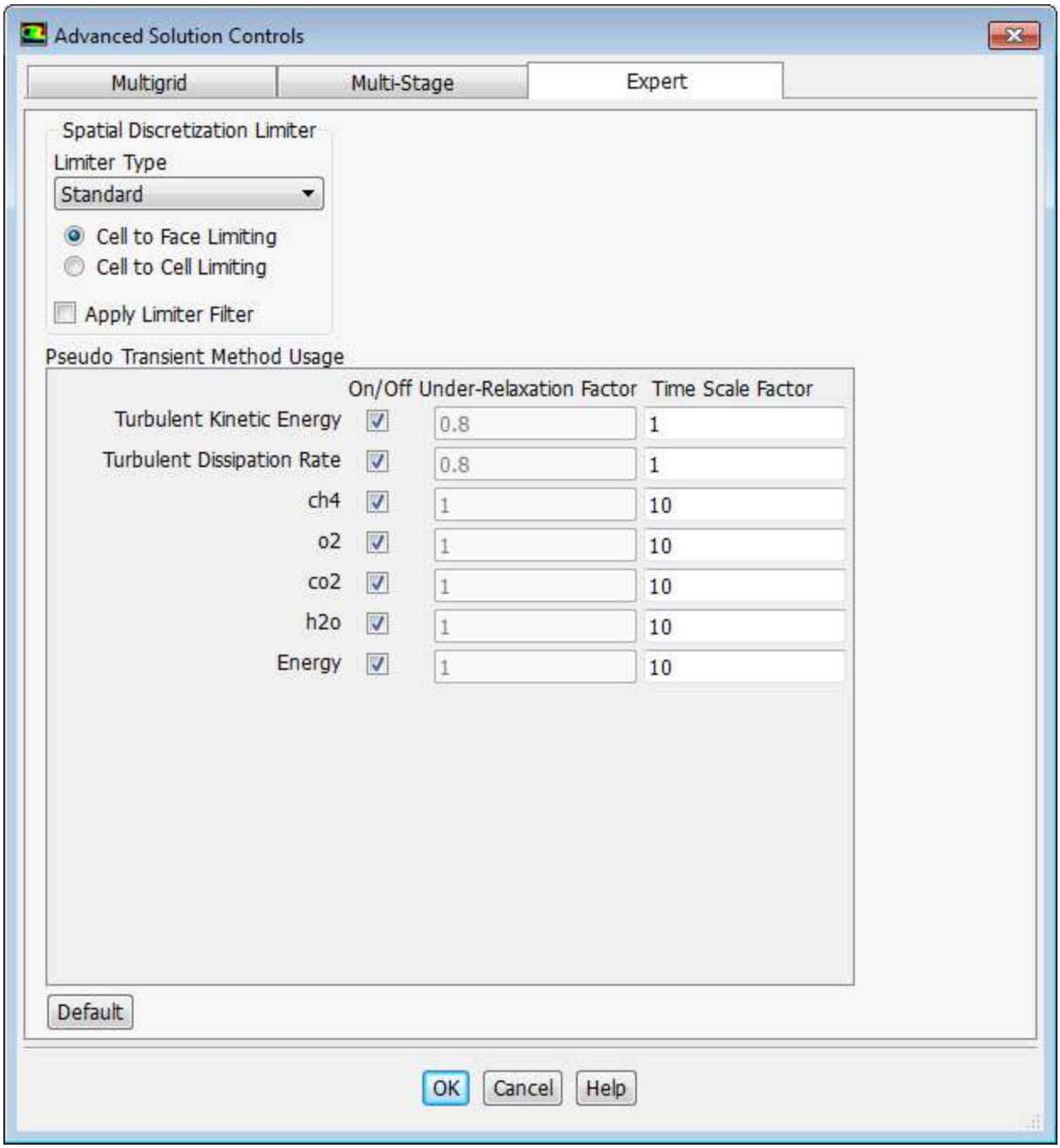


a. Enter `0.25` under **Density** in the **Pseudo Transient Explicit Relaxation Factors** group box.

   The default explicit relaxation parameters in ANSYS Fluent are appropriate for a wide range of general fluid flow problems. However, in some cases it may be necessary to reduce the relaxation factors to stabilize the solution. Some experimentation is typically necessary to establish the optimal values. For this tutorial, it is sufficient to reduce the density explicit relaxation factor to `0.25` for stability.

b. Click **Advanced...** to open the **Advanced Solution Controls** dialog box and select the **Expert** tab.

   The Expert tab in the Advanced Solution Controls dialog box allows you to individually specify the solution method and Pseudo Transient Time Scale Factors for each equation, except for the flow equations. When using the Pseudo Transient method for general reacting flow cases, increasing the species and energy time scales is recommended.



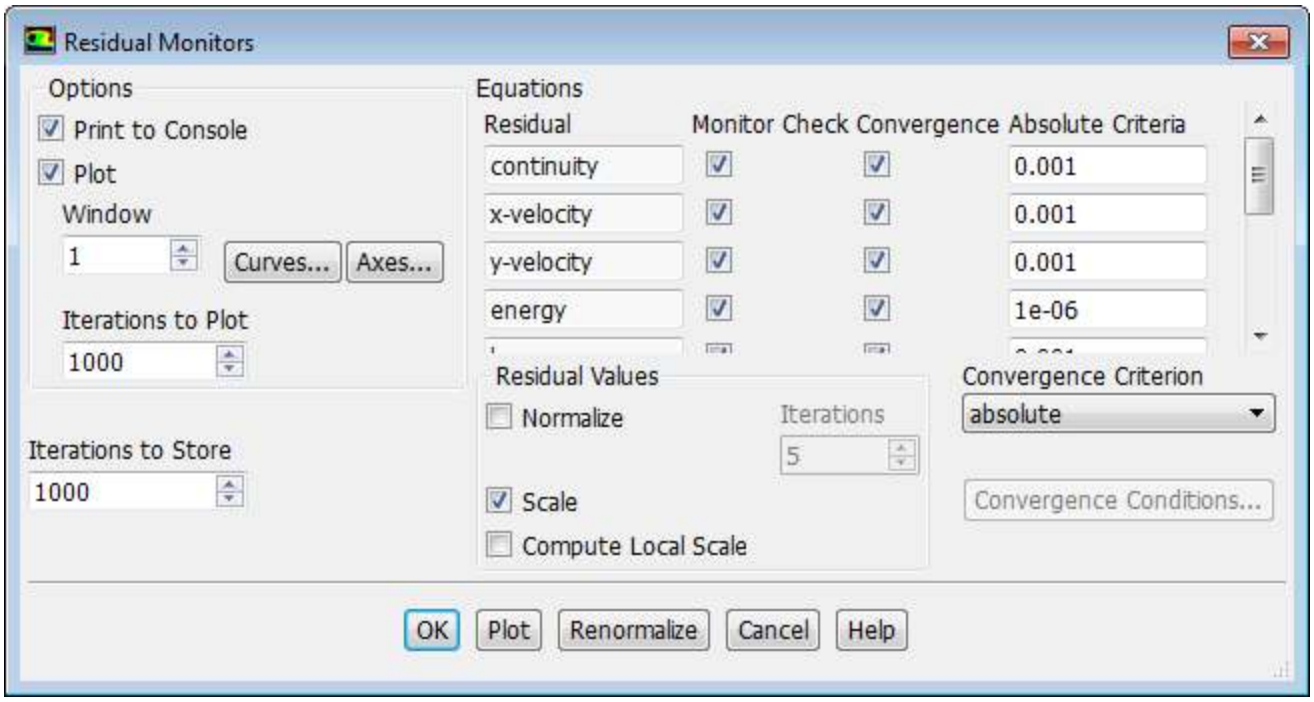
i. Enable the pseudo-transient method for **ch4**, **o2**, **co2**, **h2o**, and **Energy** in the **Expert** tab, by selecting each one under **On/Off**.

ii. Enter `10` for the **Time Scale Factor** for **ch4**, **o2**, **co2**, **h2o**, and **Energy**.

iii. Click **OK** to close the **Advanced Solution Controls** dialog box.

3. Ensure the plotting of residuals during the calculation.

Solving → Reports → Residuals...

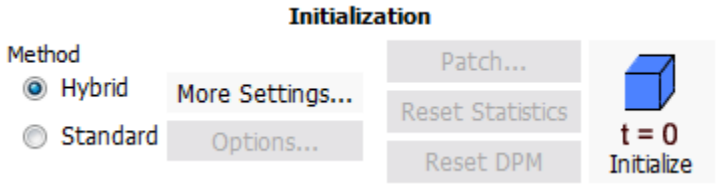


a. Ensure that **Plot** is enabled in the **Options** group box.

b. Click **OK** to close the **Residual Monitors** dialog box.

4. Initialize the field variables.

Solving → **Initialization**



a. Retain the default **Hybrid** initialization method and click **Initialize** to initialize the variables.

5. Save the case file (`gascomb1.cas.gz`).

File → **Write** → **Case...**

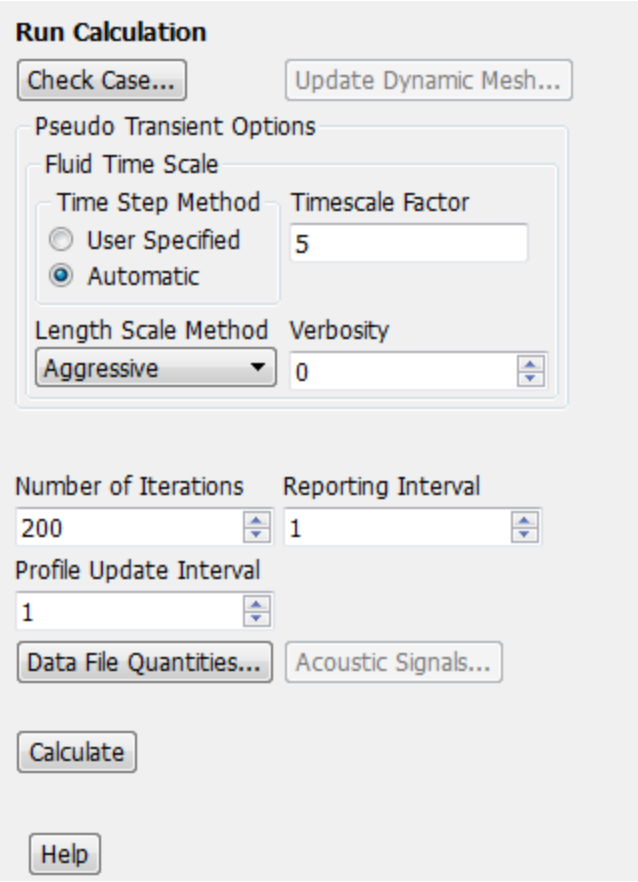
a. Enter `gascomb1.cas.gz` for **Case File**.

b. Ensure that **Write Binary Files** is enabled to produce a smaller, unformatted binary file.

c. Click **OK** to close the **Select File** dialog box.

6. Run the calculation by requesting 200 iterations.

Solving → **Run Calculation** → **Advanced...**



a. Select **Aggressive** from the **Length Scale Method** drop-down list.

   When using the Automatic Time Step Method ANSYS Fluent computes the Pseudo Transient time step based on characteristic length and velocity scales of the problem. The Conservative Length Scale Method uses the smaller of two computed length scales emphasizing solution stability. The Aggressive Length Scale Method uses the larger of the two which may provide faster convergence in some cases.

b. Enter `5` for the **Timescale Factor**.

   The Timescale Factor allows you to further manipulate the computed Time Step calculated by ANSYS Fluent. Larger time steps can lead to faster convergence. However, if the time step is too large it can lead to solution instability.

c. Enter `200` for **Number of Iterations**.

d. Click **Calculate**.

The solution will converge after approximately 160 iterations.

7. Save the case and data files (`gascomb1.cas.gz` and `gascomb1.dat.gz`).

File → Write → Case & Data...

Note

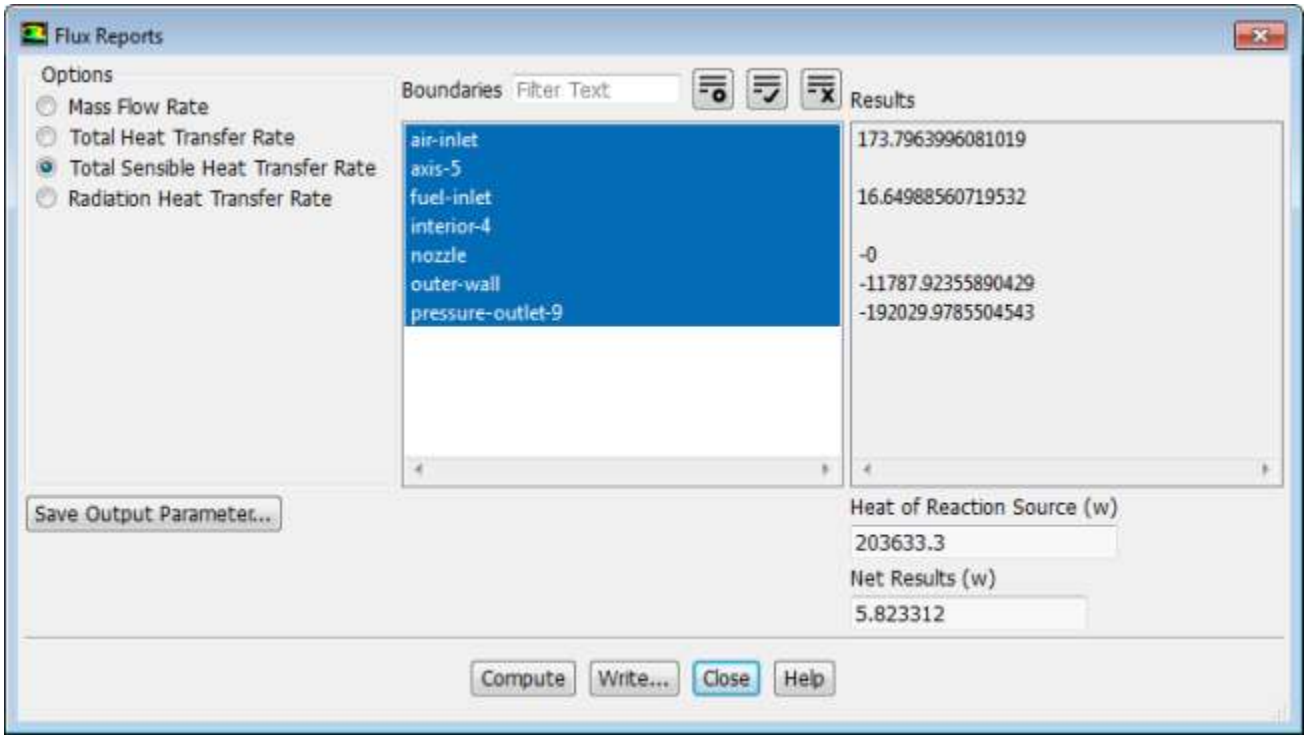
If you choose a file name that already exists in the current folder, ANSYS Fluent will ask you to confirm that the previous file is to be overwritten.

13.5.8. Postprocessing

Review the solution by examining graphical displays of the results and performing surface integrations at the combustor exit.

1. Report the total sensible heat flux.

Postprocessing → Reports → Fluxes...



a. Select **Total Sensible Heat Transfer Rate** in the **Options** list.

b. Select all the boundaries from the **Boundaries** selection list (you can click the select-all button ( ).

c. Click **Compute** and close the **Flux Reports** dialog box.

Note

The energy balance is good because the net result is small compared to the heat of reaction.

2. Display filled contours of temperature (Figure 13.3: Contours of Temperature (p. 561)).

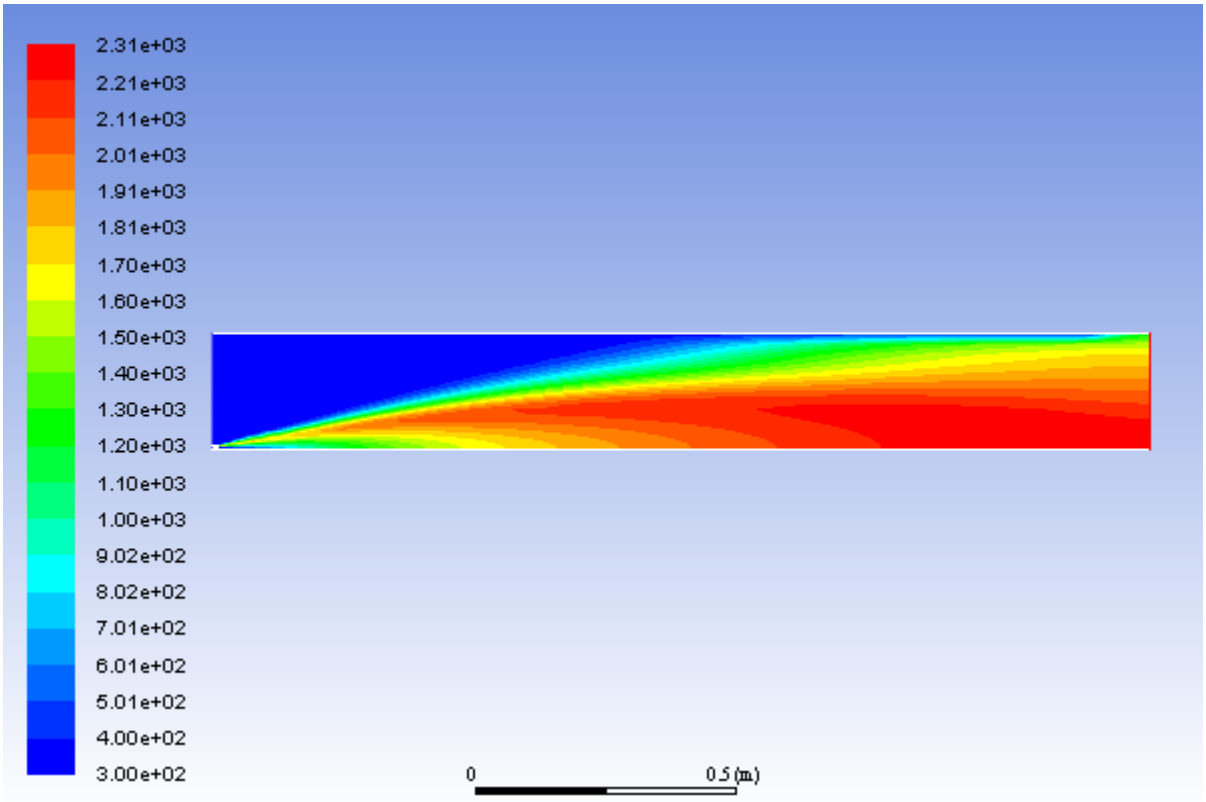
   Postprocessing → Graphics → Contours → Edit...

   a. Ensure that **Filled** is enabled in the **Options** group box.

   b. Select **Temperature...** and **Static Temperature** in the **Contours of** drop-down lists.

   c. Click **Display**.

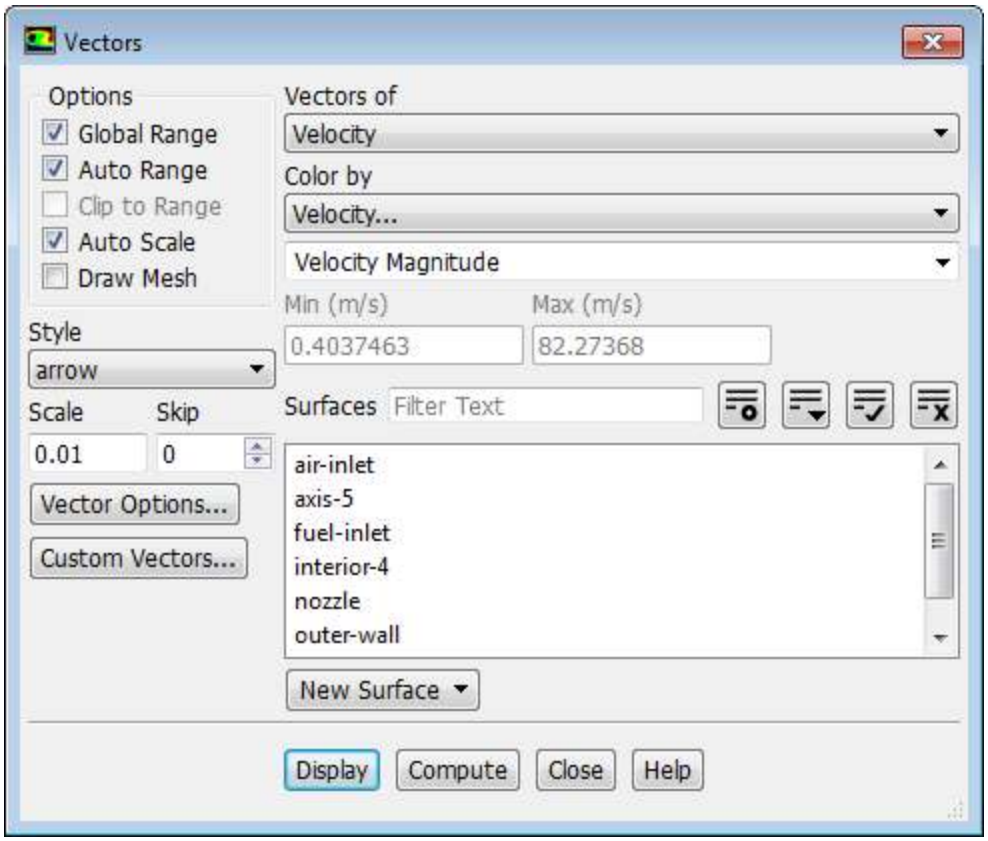
   Figure 13.3: Contours of Temperature



   The peak temperature is approximately 2310 K.

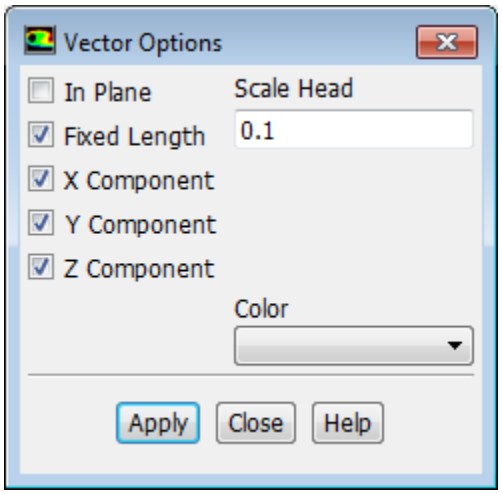
3. Display velocity vectors (Figure 13.4: Velocity Vectors (p. 563)).

   Postprocessing → Graphics → Vectors → Edit...



a. Enter `0.01` for **Scale**.

b. Click the **Vector Options...** button to open the **Vector Options** dialog box.



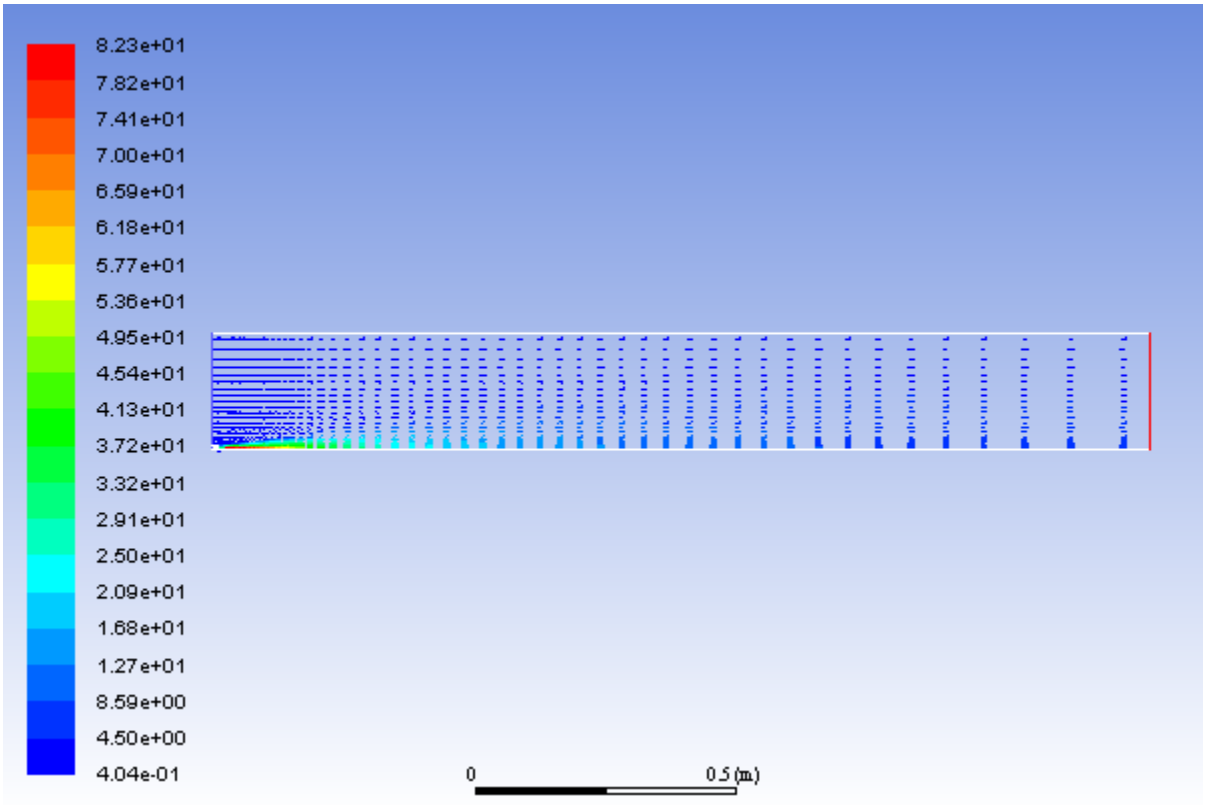
i. Enable **Fixed Length**.

The fixed length option is useful when the vector magnitude varies dramatically. With fixed length vectors, the velocity magnitude is described only by color instead of by both vector length and color.

ii. Click **Apply** and close the **Vector Options** dialog box.

c. Click **Display** and close the **Vectors** dialog box.

Figure 13.4: Velocity Vectors



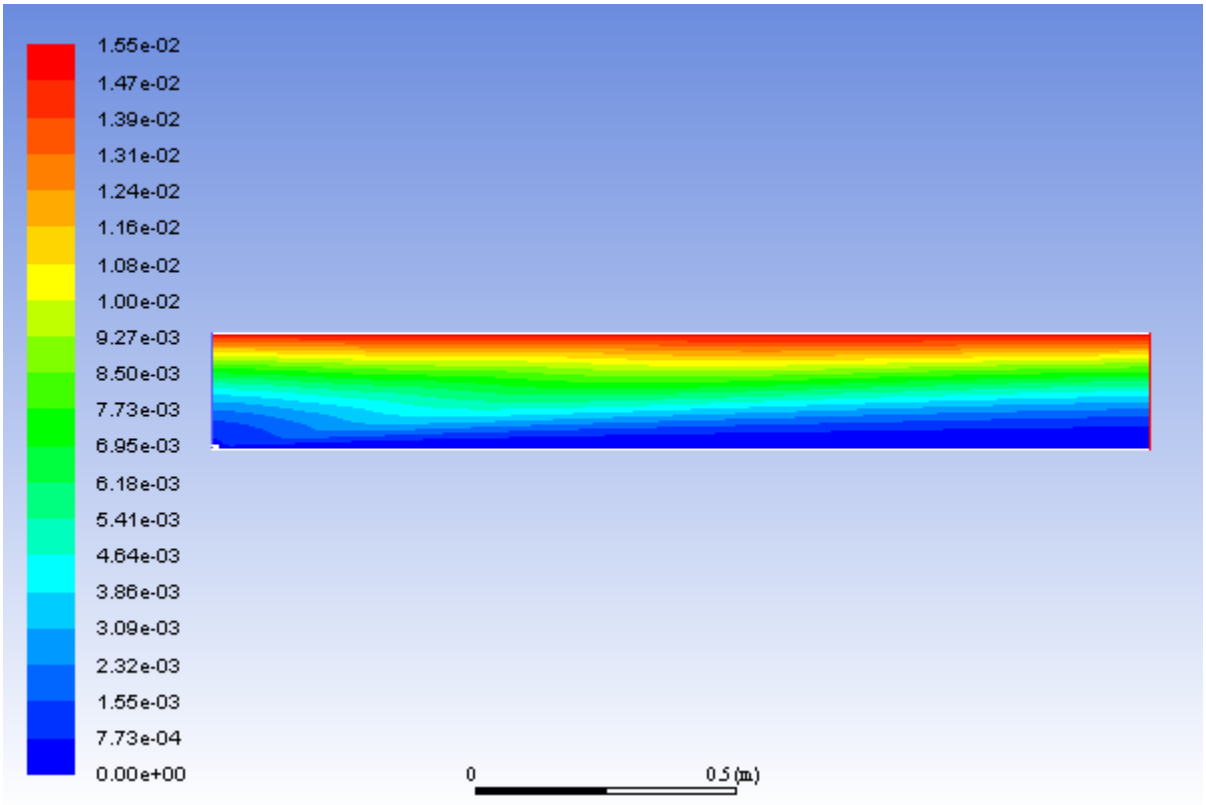
4. Display filled contours of stream function (Figure 13.5: Contours of Stream Function (p. 564)).

   Postprocessing → **Graphics** → **Contours** → **Edit...**

   a. Select **Velocity...** and **Stream Function** from the **Contours of** drop-down lists.

   b. Click **Display**.

Figure 13.5: Contours of Stream Function



The entrainment of air into the high-velocity methane jet is clearly visible in the streamline display.

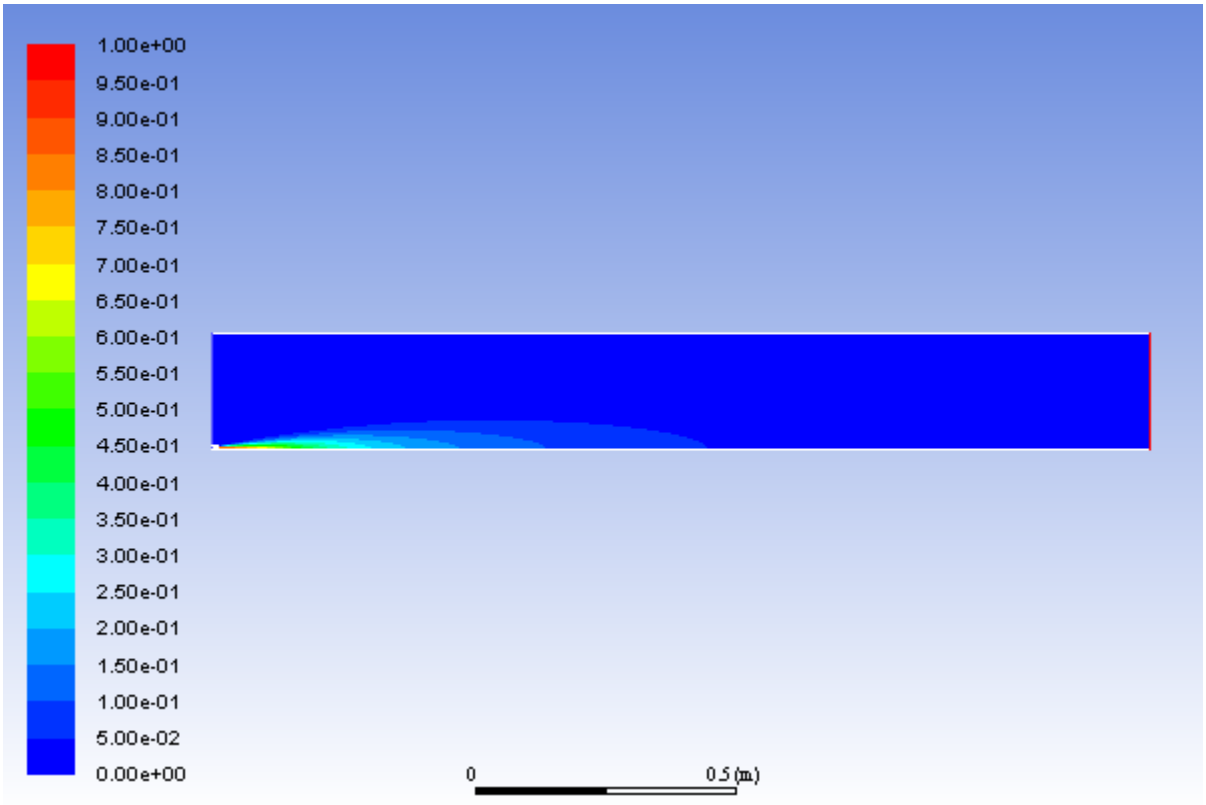
5. Display filled contours of mass fraction for CH_4 (Figure 13.6: Contours of CH4 Mass Fraction (p. 565)).

   Postprocessing → **Graphics** → **Contours** → **Edit...**

   a. Select **Species...** and **Mass fraction of ch4** from the **Contours of** drop-down lists.

   b. Click **Display**.

Figure 13.6: Contours of CH4 Mass Fraction



6. In a similar manner, display the contours of mass fraction for the remaining species O_2, CO_2, and H_2O (Figure 13.7: Contours of O2 Mass Fraction (p. 566), Figure 13.8: Contours of CO2 Mass Fraction (p. 566), and Figure 13.9: Contours of H2O Mass Fraction (p. 567)) Close the **Contours** dialog box when all of the species have been displayed.

Figure 13.7: Contours of O2 Mass Fraction

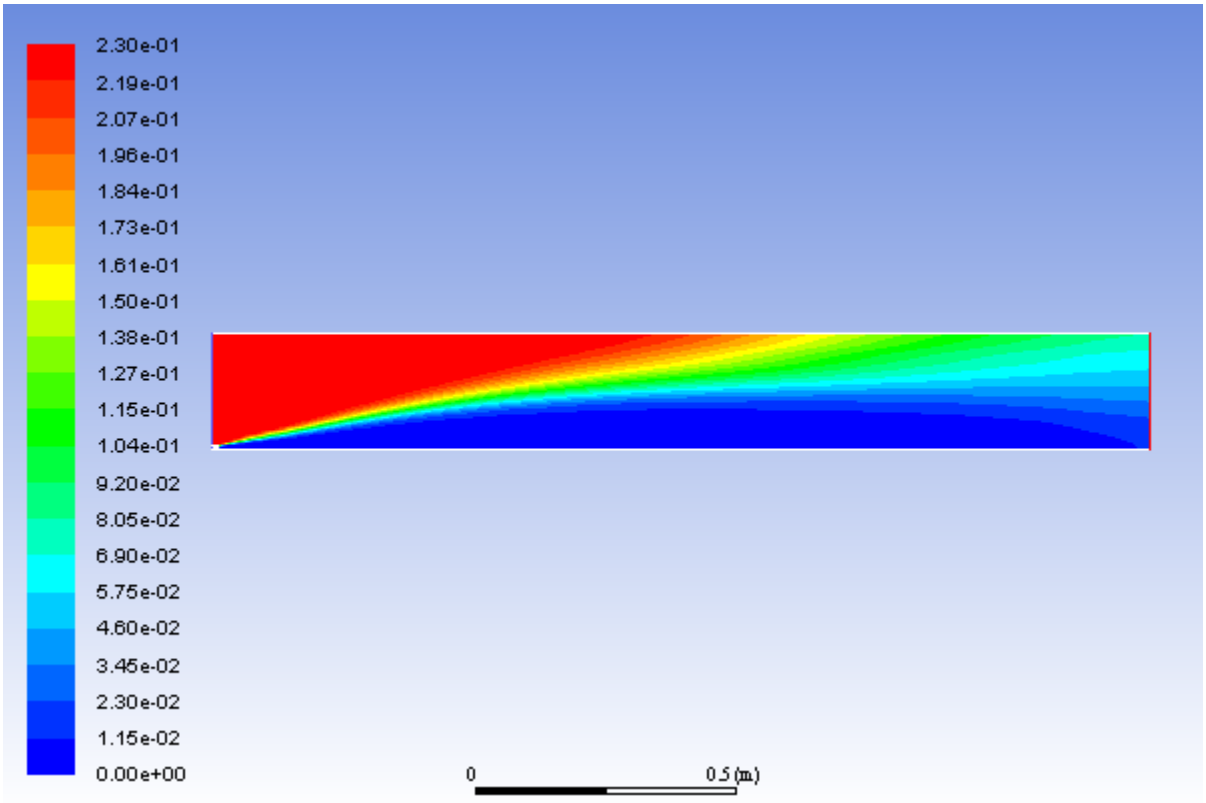


Figure 13.8: Contours of CO2 Mass Fraction

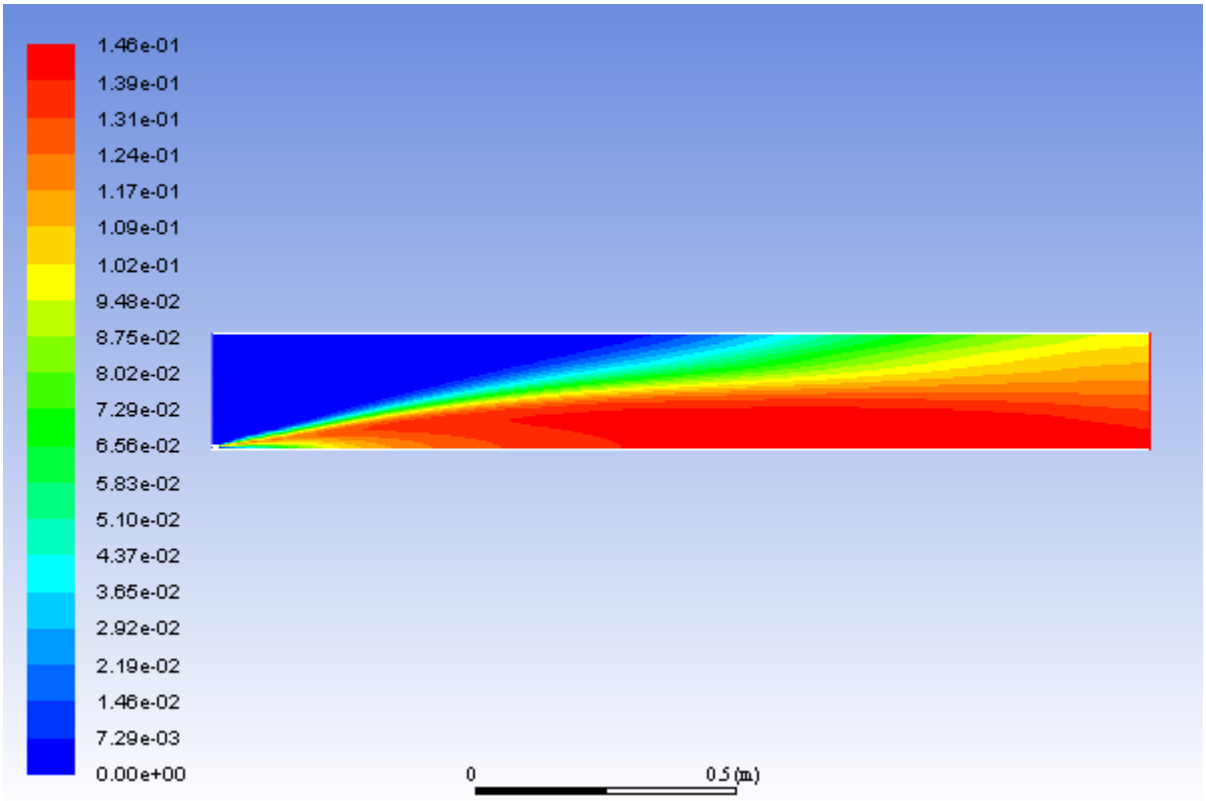
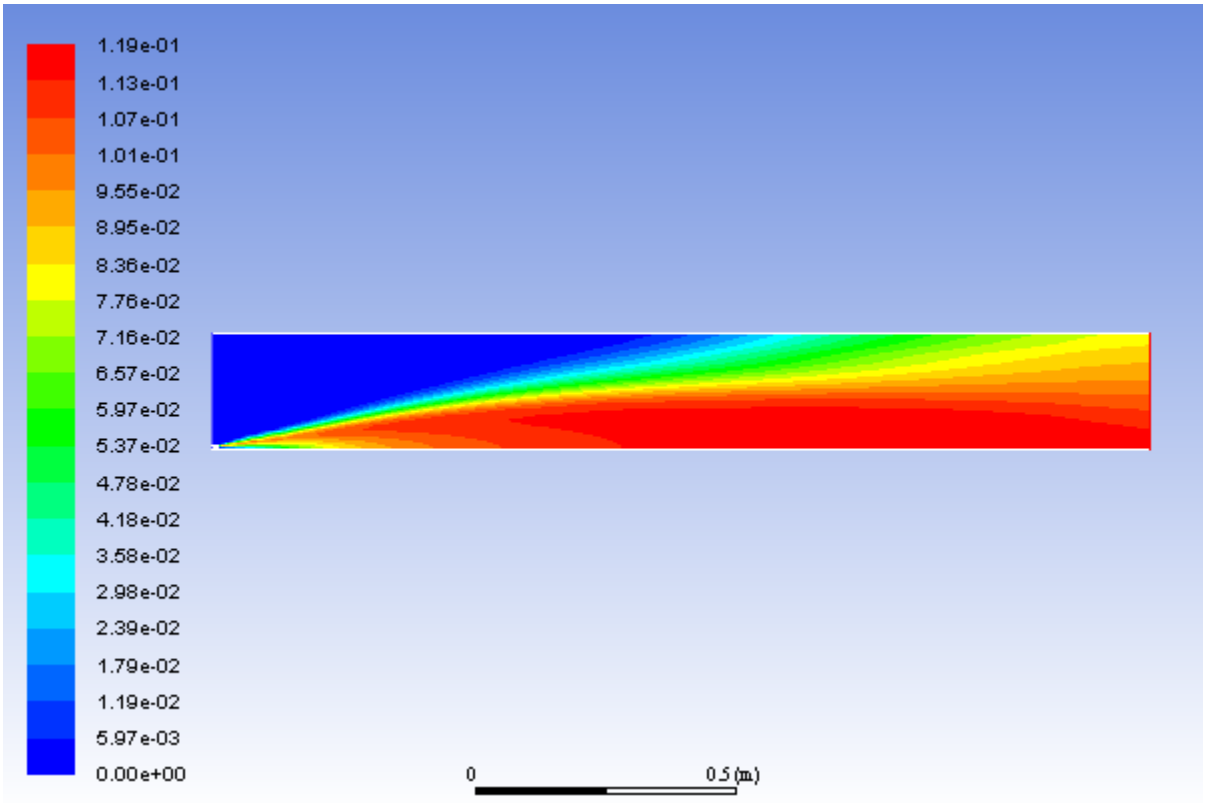
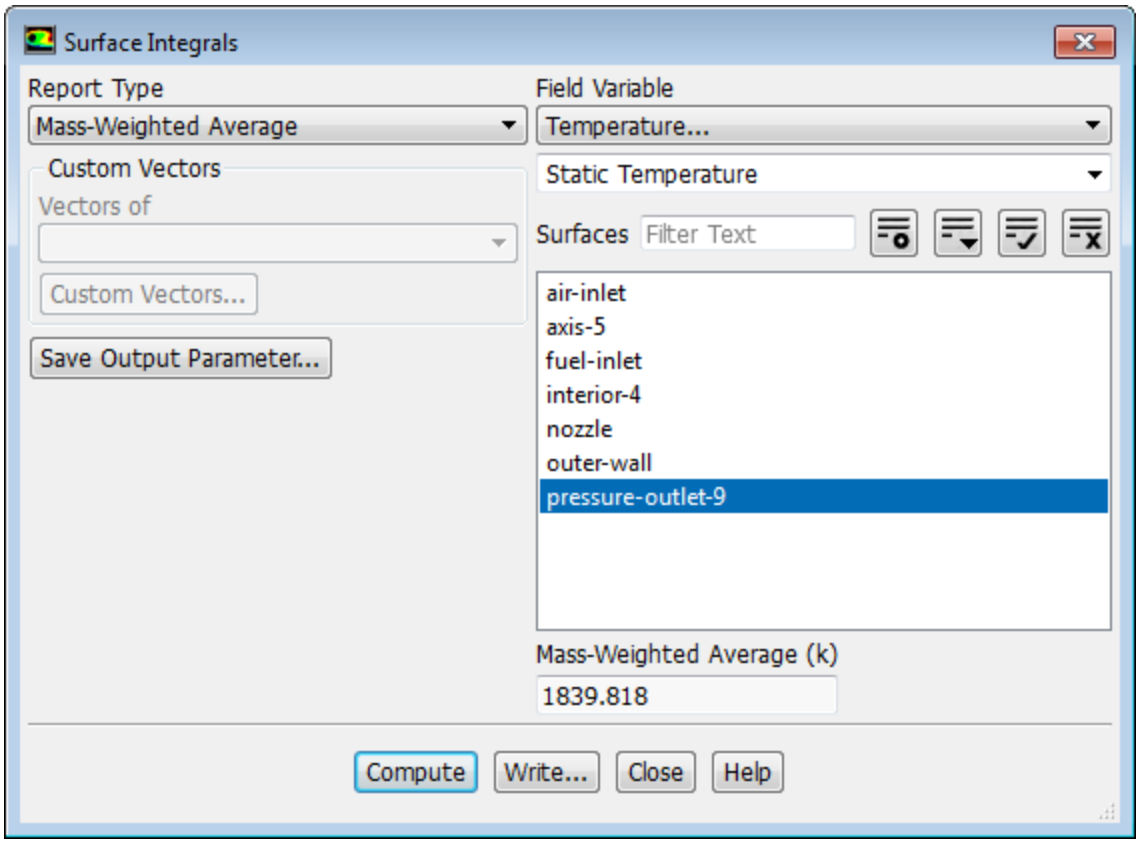


Figure 13.9: Contours of H2O Mass Fraction



7. Determine the average exit temperature.

Postprocessing → Reports → Surface Integrals...



a. Select **Mass-Weighted Average** from the **Report Type** drop-down list.

b. Select **Temperature...** and **Static Temperature** from the **Field Variable** drop-down lists.

The mass-averaged temperature will be computed as:

$$\overline{T} = \frac{\int T\rho\vec{v}\cdot d\vec{A}}{\int \rho\vec{v}\cdot d\vec{A}} \tag{13.2}$$

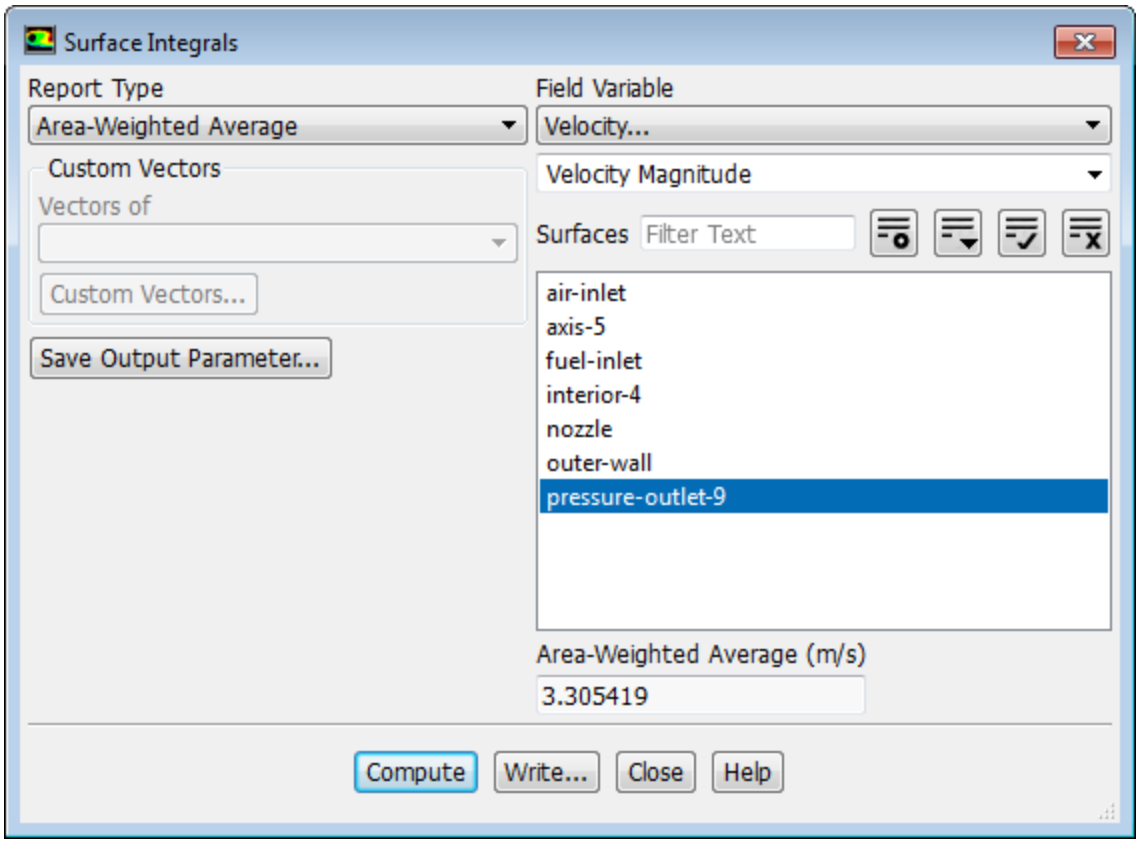
c. Select **pressure-outlet-9** from the **Surfaces** selection list, so that the integration is performed over this surface.

d. Click **Compute**.

*The **Mass-Weighted Average** field will show that the exit temperature is approximately 1840 K.*

8. Determine the average exit velocity.

Postprocessing → Reports → Surface Integrals...



a. Select **Area-Weighted Average** from the **Report Type** drop-down list.

b. Select **Velocity...** and **Velocity Magnitude** from the **Field Variable** drop-down lists.

The area-weighted velocity-magnitude average will be computed as:

$$\overline{v}=\frac{1}{A}\int vdA \tag{13.3}$$

c. Click **Compute**.

*The **Area-Weighted Average** field will show that the exit velocity is approximately 3.30 m/s.*

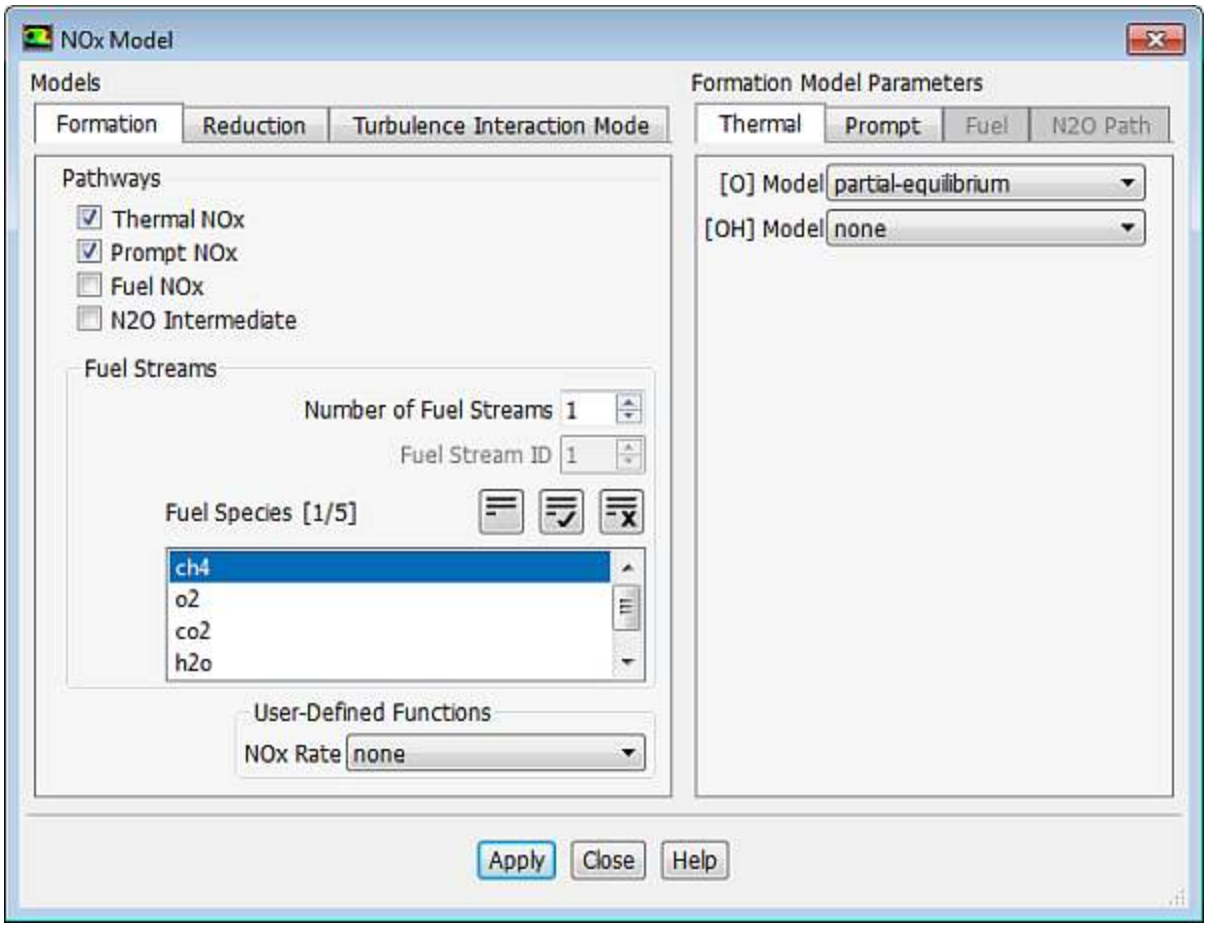
d. Close the **Surface Integrals** dialog box.

13.5.9. NOx Prediction

In this section you will extend the ANSYS Fluent model to include the prediction of NOx. You will first calculate the formation of both thermal and prompt NOx, then calculate each separately to determine the contribution of each mechanism.

1. Enable the NOx model.

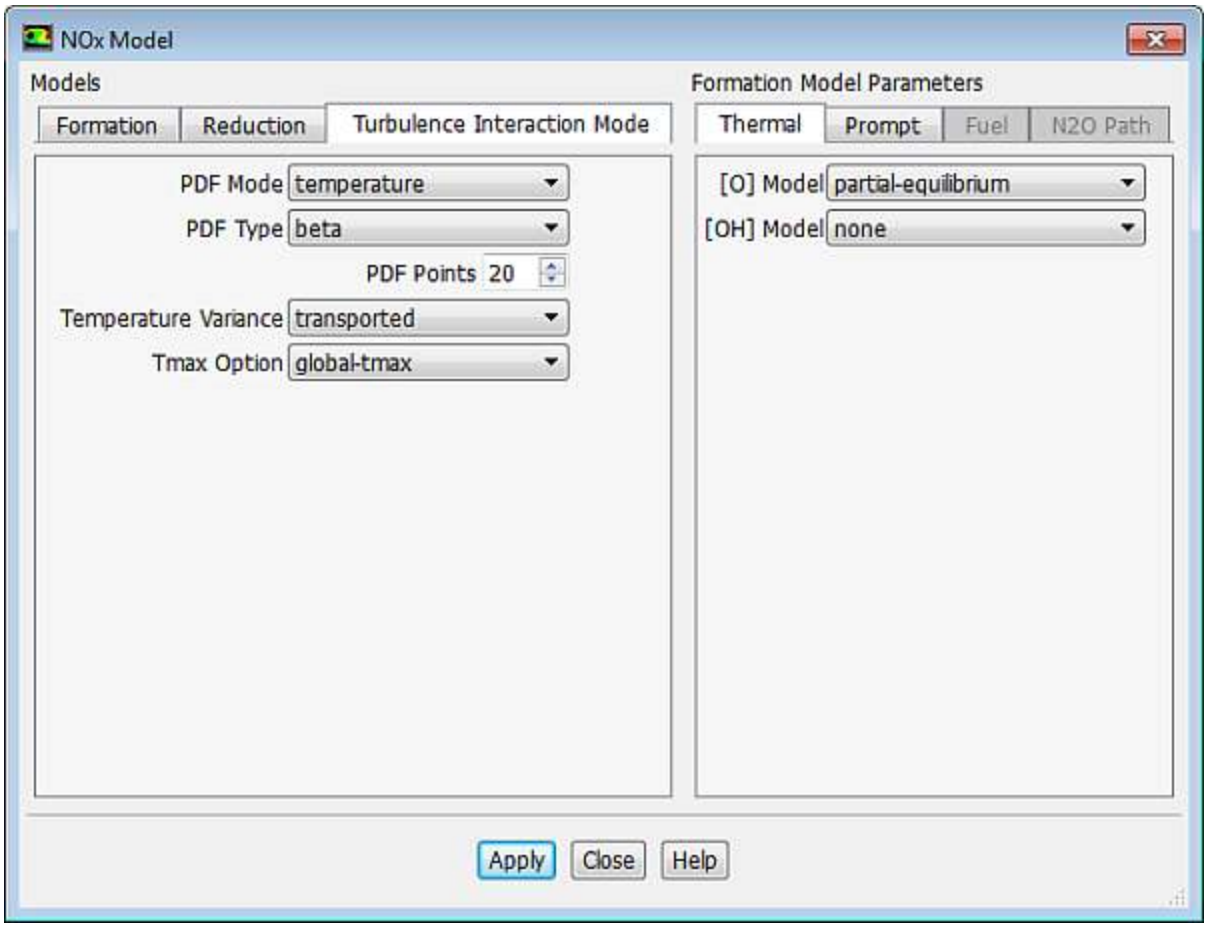
Setup → Models → Species → NOx Edit...



a. Enable **Thermal NOx** and **Prompt NOx** in the **Pathways** group box.

b. Select **ch4** from the **Fuel Species** selection list.

c. Click the **Turbulence Interaction Mode** tab.



i. Select **temperature** from the **PDF Mode** drop-down list.

This will enable the turbulence-chemistry interaction. If turbulence interaction is not enabled, you will be computing NOx formation without considering the important influence of turbulent fluctuations on the time-averaged reaction rates.

ii. Retain the default selection of **beta** from the **PDF Type** drop-down list and enter `20` for **PDF Points**.

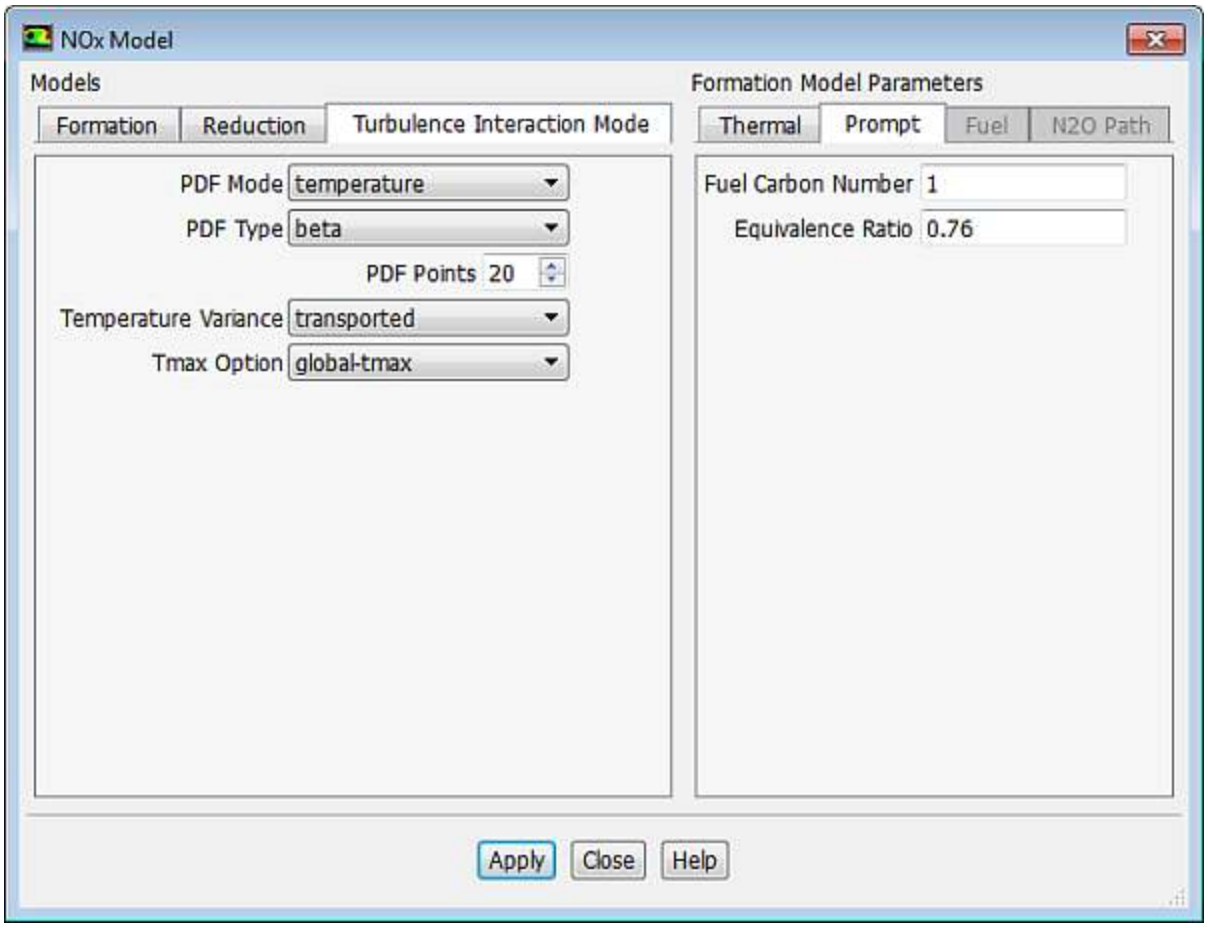
*The value for **PDF Points** is increased from `10` to `20` to obtain a more accurate NOx prediction.*

iii. Select **transported** from the **Temperature Variance** drop-down list.

d. Select **partial-equilibrium** from the **[O] Model** drop-down list in the **Formation Model Parameters** group box in the **Thermal** tab.

The partial-equilibrium model is used to predict the O radical concentration required for thermal NOx prediction.

e. Click the **Prompt** tab.



i. Retain the default value of `1` for **Fuel Carbon Number**.

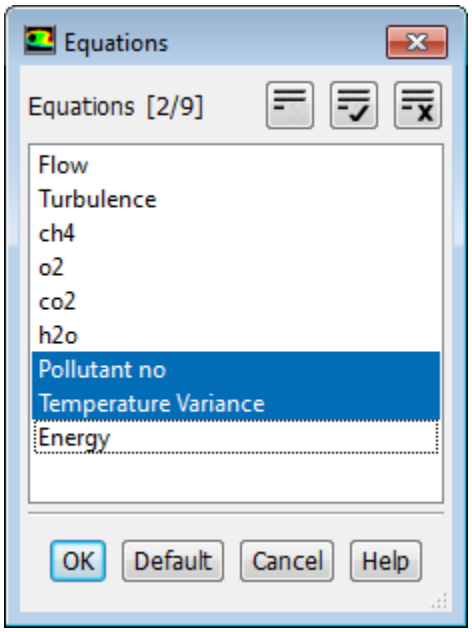
ii. Enter `0.76` for **Equivalence Ratio**.

*All of the parameters in the **Prompt** tab are used in the calculation of prompt NOx formation. The **Fuel Carbon Number** is the number of carbon atoms per molecule of fuel. The **Equivalence Ratio** defines the fuel-air ratio (relative to stoichiometric conditions).*

f. Click **Apply** to accept these changes and close the **NOx Model** dialog box.

2. Enable the calculation of NO species only and temperature variance.

Solving → Controls → Equations...



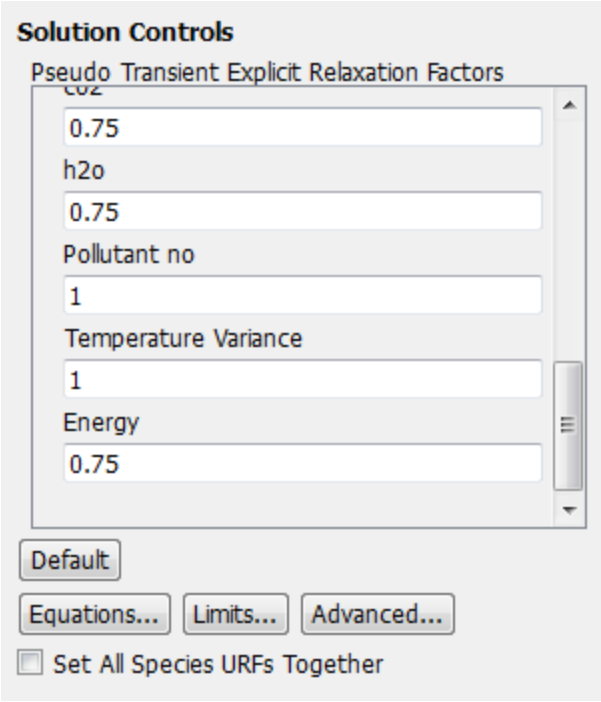
a. Deselect all variables except **Pollutant no** and **Temperature Variance** from the **Equations** selection list.

b. Click **OK** to close the **Equations** dialog box.

You will predict NOx formation in a "postprocessing" mode, with the flow field, temperature, and hydrocarbon combustion species concentrations fixed. Hence, only the NO equation will be computed. Prediction of NO in this mode is justified on the grounds that the NO concentrations are very low and have negligible impact on the hydrocarbon combustion prediction.

3. Modify the solution controls for **Pollutant no** and **Temperature Variance**.

Solving → Controls → Controls...



a. Click **Advanced...** to open the **Advanced Solution Controls** dialog box.

i. In the **Expert** tab, enable the pseudo-transient method for **Pollutant no** and **Temperature Variance**, by selecting them under **On/Off**.

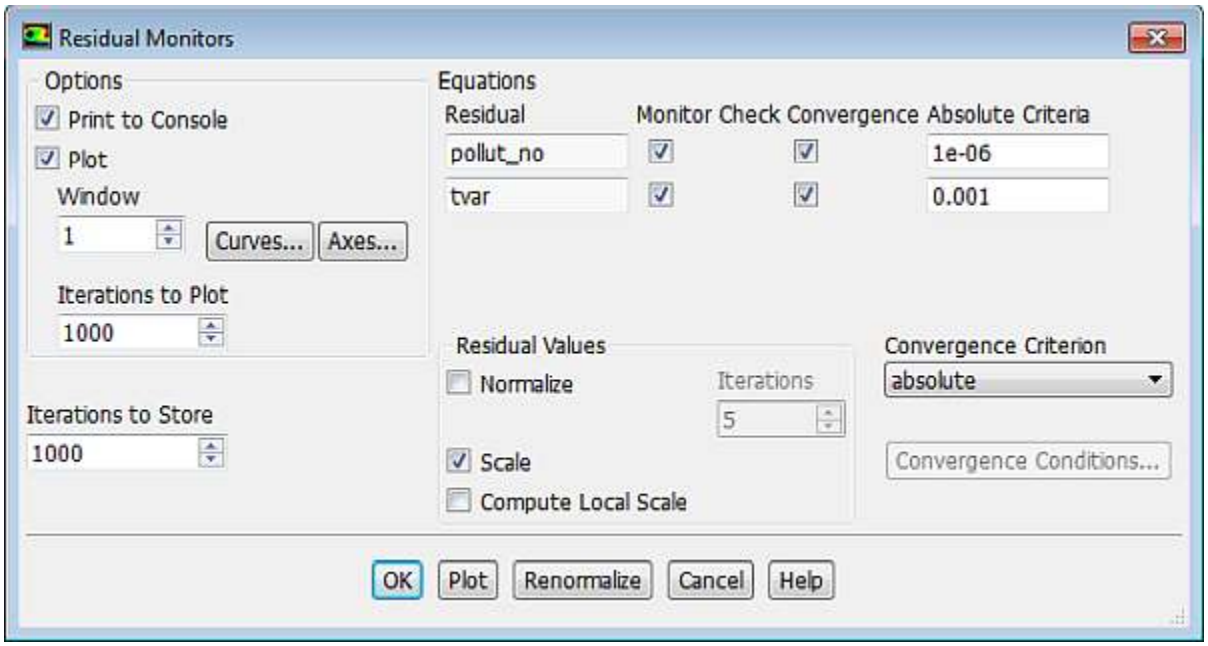
ii. Enter `10` for **Time Scale Factor** for **Pollutant no** and **Temperature Variance**.

iii. Click **OK** to close the **Advanced Solution Controls** dialog box.

b. Enter `1` for **Pollutant no** and **Temperature Variance** in the **Pseudo Transient Explicit Relaxation Factors** group box.

4. Confirm the convergence criterion for the NO species equation.

Solving → Reports → Residuals...



a. Ensure that the **Absolute Criteria** for **pollut_no** is set to `1e-06`.

b. Click **OK** to close the **Residual Monitors** dialog box.

5. Request 25 more iterations.

Solution → Run Calculation

The solution will converge in approximately 10 iterations.

6. Save the new case and data files (`gascomb2.cas.gz` and `gascomb2.dat.gz`).

File → Write → Case & Data...

7. Review the solution by creating and displaying a contour definition for NO mass fraction (Figure 13.10: Contours of NO Mass Fraction — Prompt and Thermal NOx Formation (p. 575)).

Postprocessing → Graphics → Contours → New...

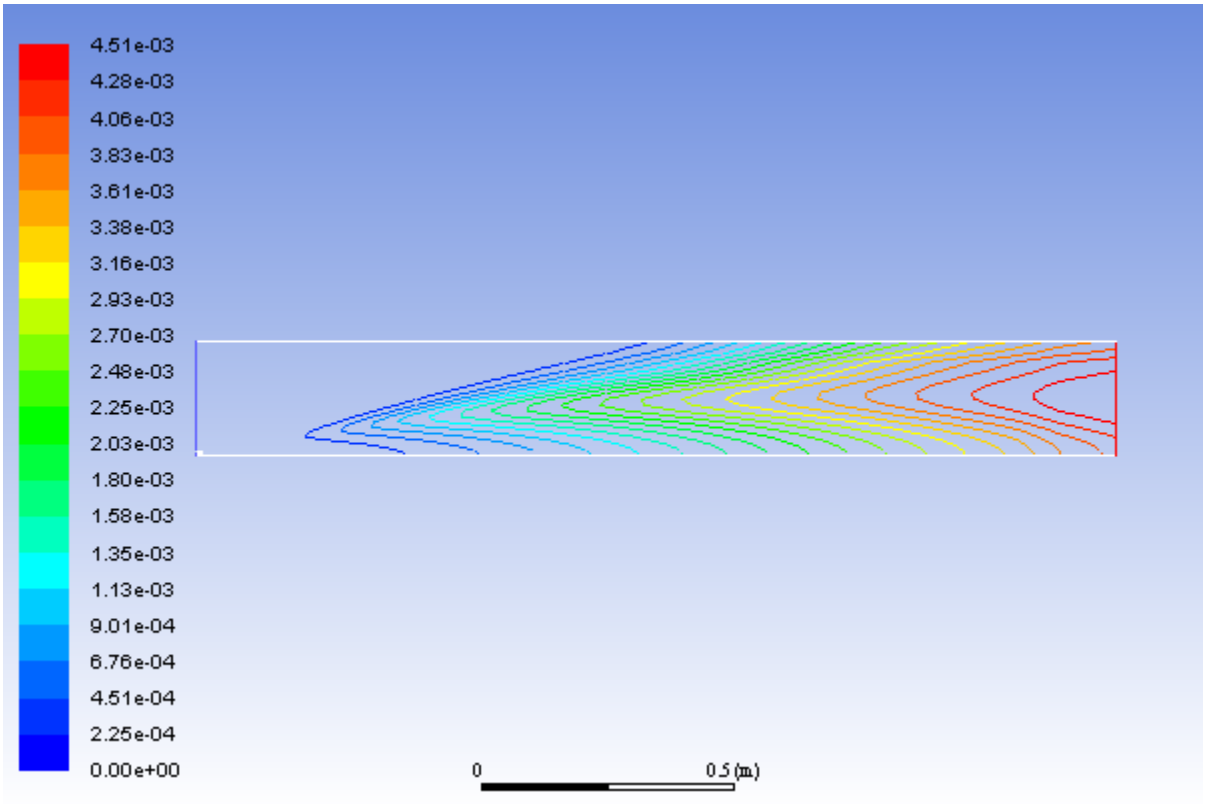
a. Enter **contour-no-mass-fraction** for **Contour Name**.

b. Disable **Filled** in the **Options** group box.

c. Select **NOx...** and **Mass fraction of Pollutant no** from the **Contours of** drop-down lists.

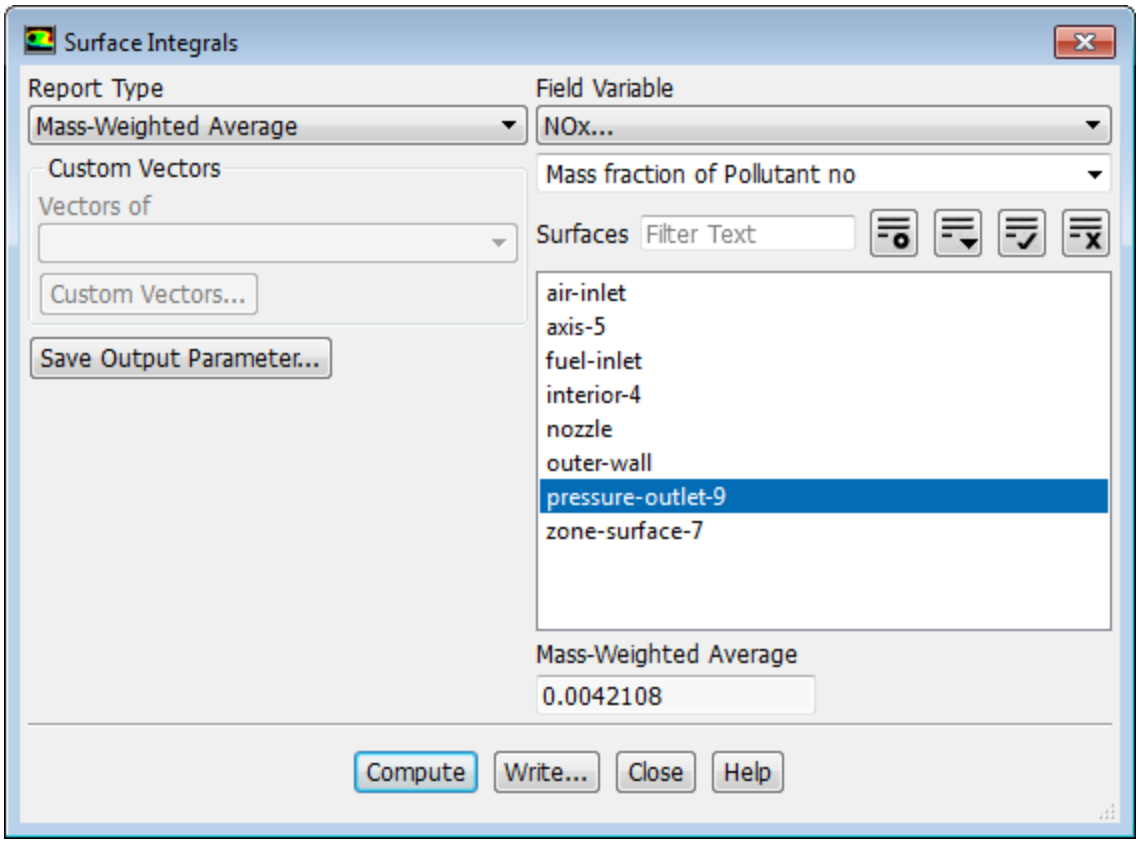
d. Click **Save/Display** and close the **Contours** dialog box.

Figure 13.10: Contours of NO Mass Fraction — Prompt and Thermal NOx Formation



8. Calculate the average exit NO mass fraction.

Postprocessing → Reports → Surface Integrals...



a. Select **Mass-Weighted Average** from the **Report Type** drop-down list.

b. Select **NOx...** and **Mass fraction of Pollutant no** from the **Field Variable** drop-down lists.

c. Ensure that **pressure-outlet-9** is selected from the **Surfaces** selection list.

d. Click **Compute**.

*The **Mass-Weighted Average** field will show that the exit NO mass fraction is approximately 0.00421.*

e. Close the **Surface Integrals** dialog box.

9. Disable the prompt NOx mechanism in preparation for solving for thermal NOx only.

Setup → Models → Species → NOx Edit...

a. In the **Formation** tab, disable **Prompt NOx**.

b. Click **Apply** and close the **NOx Model** dialog box.

10. Request 25 iterations.

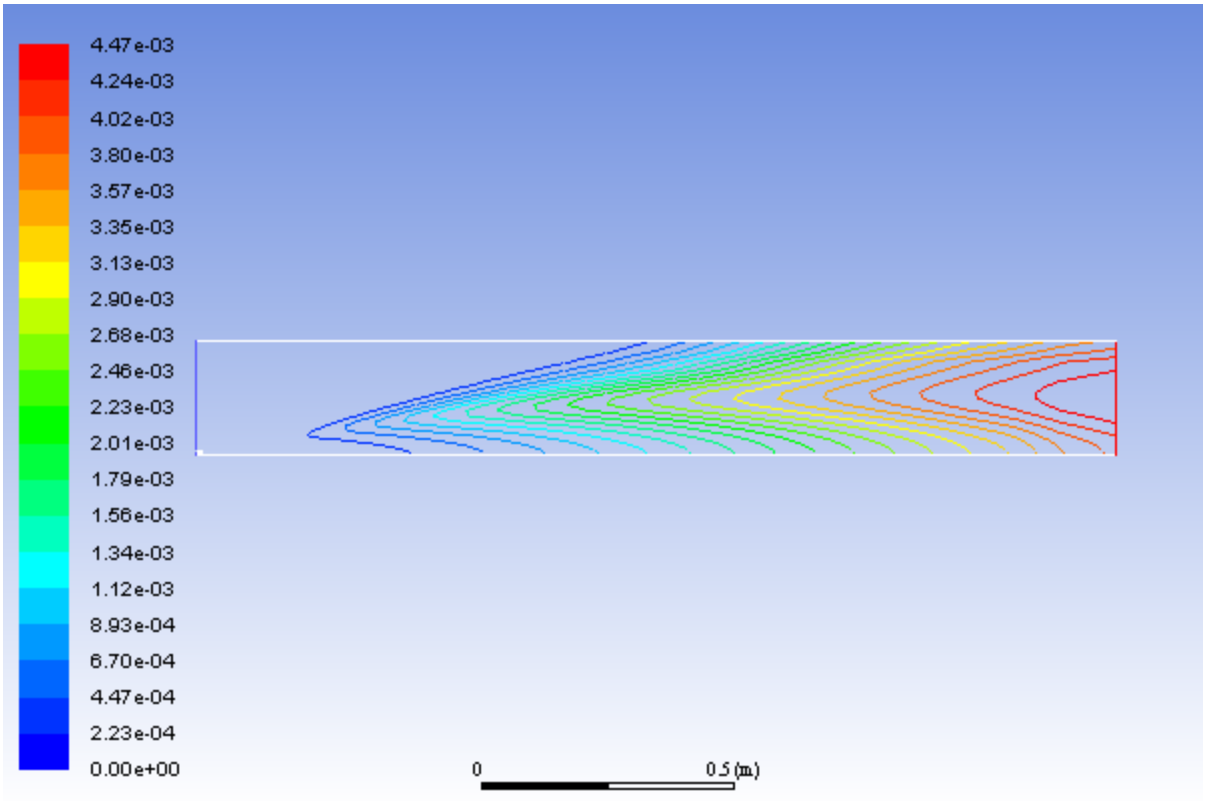
Solution → Run Calculation

The solution will converge in approximately 6 iterations.

11. Review the thermal NOx solution by displaying the **contour-no-mass-fraction** contour definition for NO mass fraction (under the **Results/Graphics/Contours** tree branch) you created earlier (Figure 13.11: Contours of NO Mass Fraction—Thermal NOx Formation (p. 577)).

Results → Graphics → Contours → contour-no-mass-fraction → Display

Figure 13.11: Contours of NO Mass Fraction—Thermal NOx Formation



Note that the concentration of NO is slightly lower without the prompt NOx mechanism.

12. Compute the average exit NO mass fraction with only thermal NOx formation.

Postprocessing → Reports → Surface Integrals...

Tip

Follow the same procedure you used earlier for the calculation with both thermal and prompt NOx formation.

---

*The **Mass-Weighted Average** field will show that the exit NO mass fraction with only thermal NOx formation (without prompt NOx formation) is approximately 0.004174.*

13. Solve for prompt NOx production only.

Setup → Models → Species → NOx → Edit...

a. Disable **Thermal NOx** in the **Pathways** group box.

b. Enable **Prompt NOx**.

c. Click **Apply** and close the **NOx Model** dialog box.

14. Request 25 iterations.

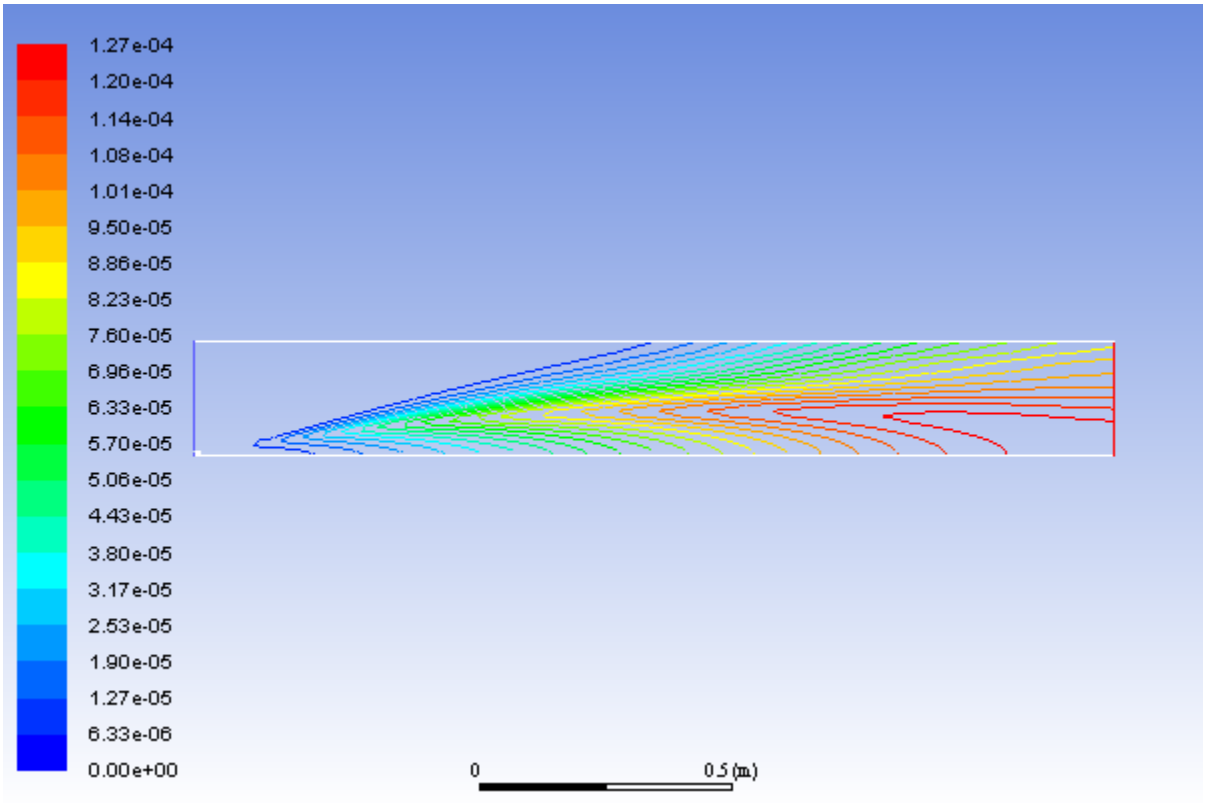
Solution → Run Calculation

The solution will converge in approximately 13 iterations.

15. Review the prompt NOx solution by displaying the **contour-no-mass-fraction** contour definition for NO mass fraction (under the **Results/Graphics/Contours** tree branch) (Figure 13.12: Contours of NO Mass Fraction—Prompt NOx Formation (p. 578)).

Results → Graphics → Contours → contour-no-mass-fraction → Display

Figure 13.12: Contours of NO Mass Fraction—Prompt NOx Formation



The prompt NOx mechanism is most significant in fuel-rich flames. In this case the flame is lean and prompt NO production is low.

16. Compute the average exit NO mass fraction only with prompt NOx formation.

Postprocessing → Reports → Surface Integrals...

Tip

Follow the same procedure you used earlier for the calculation with both thermal and prompt NOx formation.

*The **Mass-Weighted Average** field will show that the exit NO mass fraction with only prompt NOx formation is approximately 9.975e-05.*

Note

The individual thermal and prompt NO mass fractions do not add up to the levels predicted with the two models combined. This is because reversible reactions are involved. NO produced in one reaction can be destroyed in another reaction.

17. Use a custom field function to compute NO parts per million (ppm).

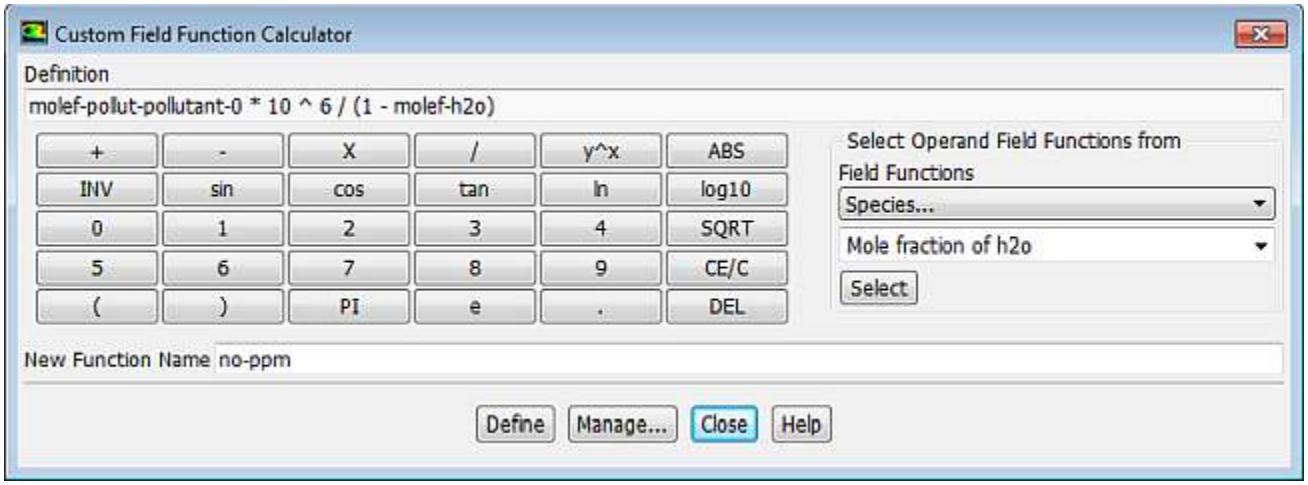
The NOppm will be computed from the following equation:

$$NOppm = \frac{NOmole fraction \times 10^6}{1 - H_2Omole fraction} \tag{13.4}$$

Note

This is the dry ppm. Therefore, the value is normalized by removing the water mole fraction in the denominator.

User Defined → Field Functions → Custom...



a. Select **NOx...** and **Mole fraction of Pollutant no** from the **Field Functions** drop-down lists, and click the **Select** button to enter **molef-pollut-pollutant-0** in the **Definition** field.

b. Click the appropriate calculator buttons to enter

```
*10^6/(1-
```

in the **Definition** field, as shown in the previous dialog box.

> **Tip**
>
> If you make a mistake, click the **DEL** button on the calculator pad to delete the last item you added to the function definition.

For more explicit instructions on using the **Custom Field Function** calculator buttons, see Introduction to Using ANSYS Fluent: Fluid Flow and Heat Transfer in a Mixing Elbow (p. 121).

c. Select **Species...** and **Mole fraction of h2o** from the **Field Functions** drop-down lists, and click the **Select** button to enter **molef-h2o** in the **Definition** field.

d. Click the **)** button to complete the field function.

e. Enter `no-ppm` for **New Function Name**.

f. Click **Define** to add the new field function to the variable list and close the **Custom Field Function Calculator** dialog box.

18. Display contours of NO ppm (Figure 13.13: Contours of NO ppm — Prompt NOx Formation (p. 581)).

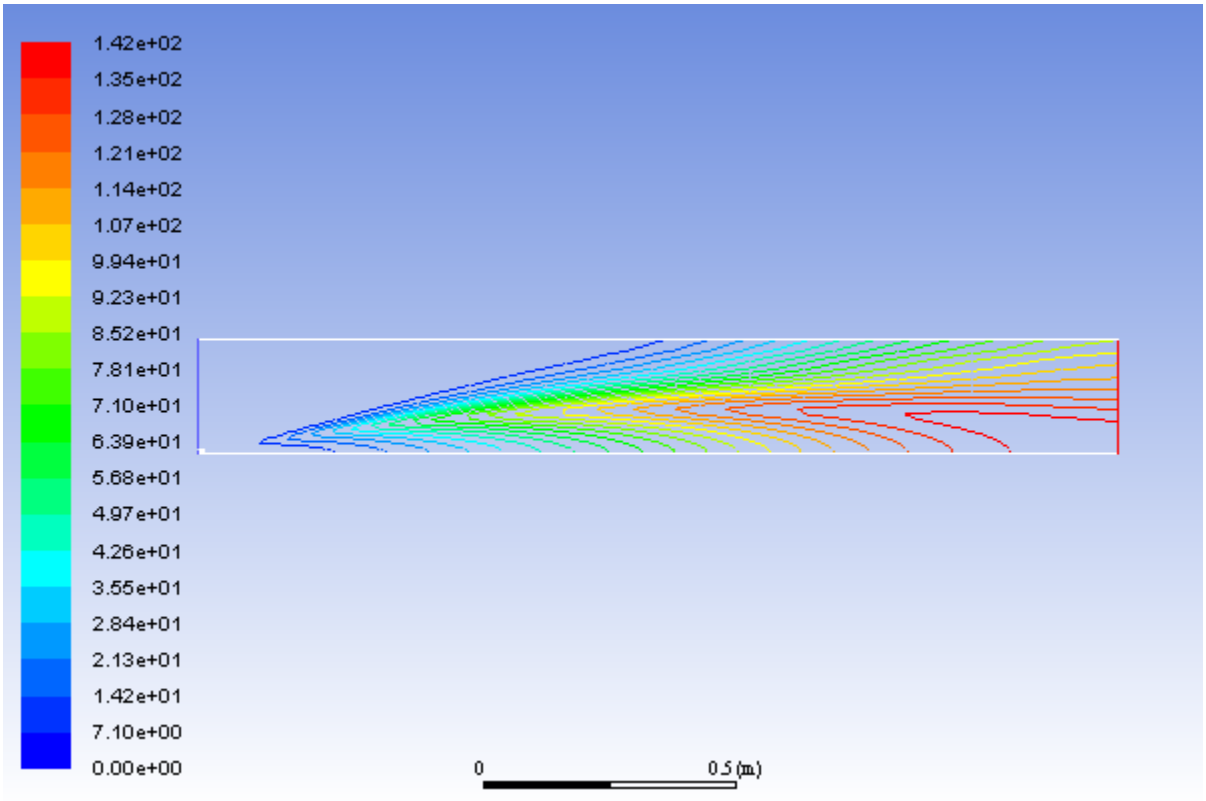
 **Postprocessing** → **Graphics** → **Contours** → **Edit...**

a. Select **Custom Field Functions...** and **no-ppm** from the **Contours of** drop-down lists.

*Scroll up the list to find **Custom Field Functions...**.*

b. Click **Display** and close the **Contours** dialog box.

Figure 13.13: Contours of NO ppm — Prompt NOx Formation



The contours closely resemble the mass fraction contours (Figure 13.12: Contours of NO Mass Fraction—Prompt NOx Formation (p. 578)), as expected.

13.6. Summary

In this tutorial you used ANSYS Fluent to model the transport, mixing, and reaction of chemical species. The reaction system was defined by using a mixture-material entry in the ANSYS Fluent database. The procedures used here for simulation of hydrocarbon combustion can be applied to other reacting flow systems.

The NOx production in this case was dominated by the thermal NO mechanism. This mechanism is very sensitive to temperature. Every effort should be made to ensure that the temperature solution is not overpredicted, since this will lead to unrealistically high predicted levels of NO.

13.7. Further Improvements

Further improvements can be expected by including the effects of intermediate species and radiation, both of which will result in lower predicted combustion temperatures.

The single-step reaction process used in this tutorial cannot account for the moderating effects of intermediate reaction products, such as CO and H_2. Multiple-step reactions can be used to address these species. If a multi-step Magnussen model is used, considerably more computational effort is required to solve for the additional species. Where applicable, the nonpremixed combustion model can be used to account for intermediate species at a reduced computational cost.

For more details on the nonpremixed combustion model, see the Fluent User's Guide.

Radiation heat transfer tends to make the temperature distribution more uniform, thereby lowering the peak temperature. In addition, radiation heat transfer to the wall can be very significant (especially here, with the wall temperature set at 300 K). The large influence of radiation can be anticipated by computing the Boltzmann number for the flow:

$$Bo = \frac{(\rho U C_p)_{inlet}}{\sigma T_{AF}^3} \sim \frac{\text{convection}}{\text{radiation}}$$

where σ is the Boltzmann constant (5.729×10^{-8} W/m^2-K^4) and T_{AF} is the adiabatic flame temperature. For a quick estimate, assume $\rho = 1$ kg/m^3, $U = 0.5$ m/s, and $C_p = 1000$ $J/kg-K$ (the majority of the inflow is air). Assume $T_{AF} = 2000$ K. The resulting Boltzmann number is Bo = 1.09, which shows that radiation is of approximately equal importance to convection for this problem.

For details on radiation modeling, see the Fluent User's Guide.

This tutorial guides you through the steps to reach an initial set of solutions. You may be able to obtain a more accurate solution by using an appropriate higher-order discretization scheme and by adapting the mesh. Mesh adaption can also ensure that the solution is independent of the mesh. These steps are demonstrated in Introduction to Using ANSYS Fluent: Fluid Flow and Heat Transfer in a Mixing Elbow (p. 121).