Tutorial 14. Modeling Species Transport and Gaseous Combustion

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.
- Compare the results computed with constant and variable specific heat.
- Examine the reacting flow results using graphics.
- Predict thermal and prompt NO_x production.
- Use custom field functions to compute NO parts per million.

Prerequisites

This tutorial is written with the assumption that you have completed Tutorial 1, 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.

To learn more about chemical reaction modeling, see Chapter 15 in the separate User's Guide and Chapter 7 in the separate Theory Guide. Otherwise, no previous experience with chemical reaction or combustion modeling is assumed.

Problem Description

The cylindrical combustor considered in this tutorial is shown in Figure 14.1. 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.

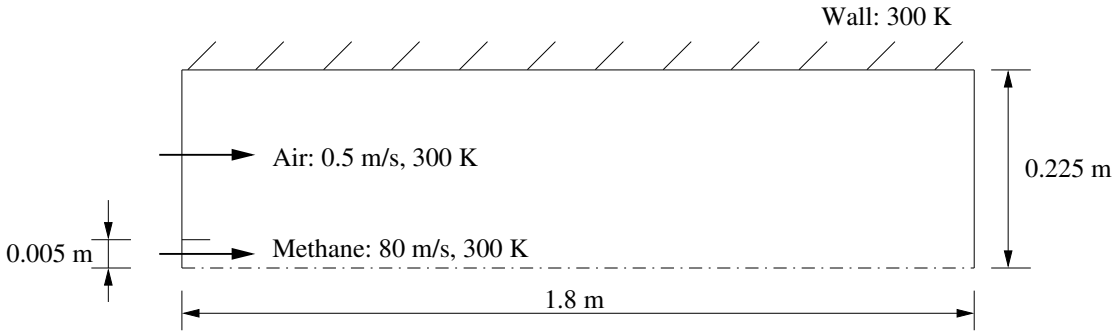


Figure 14.1: Combustion of Methane Gas in a Turbulent Diffusion Flame Furnace

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

$$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O \tag{14.1}$$

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.

Setup and Solution

Preparation

1. Download `species_transport.zip` from the User Services Center to your working folder (as described in Tutorial 1).

2. Unzip `species_transport.zip`.

   The file `gascomb.msh` *can be found in the* `species_transport` *folder created after unzipping the file.*

3. Use FLUENT Launcher to start the 2D version of ANSYS FLUENT.

   For more information about FLUENT Launcher*, see Section 1.1.2 in the separate User's Guide.*

4. Enable Double-Precision.

Note: *The* Display Options *are enabled by default. Therefore, after you read in the mesh, it will be displayed in the embedded graphics window.*

Step 1: 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.*

Step 2: General Settings

General

1. Check the mesh.

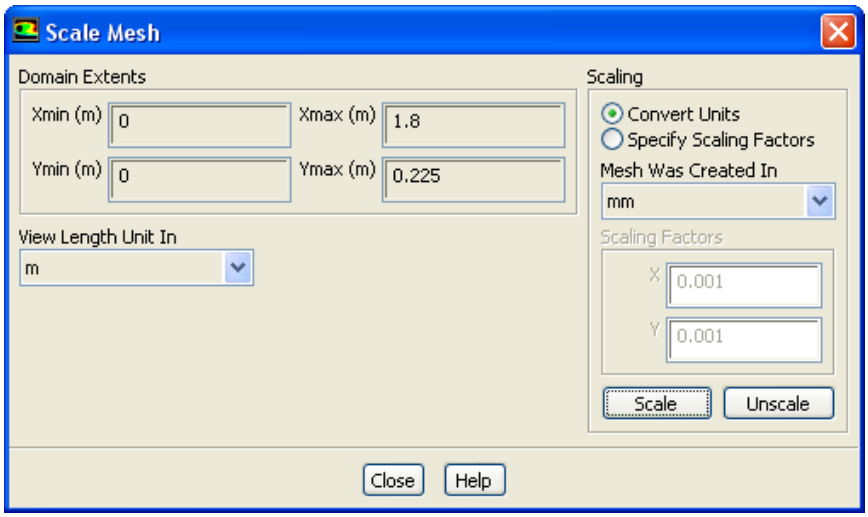
   General → Check

   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.

   General → 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 set 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.

   General → Check

   Note: *It is a good practice to check the mesh after you manipulate it (i.e., 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.

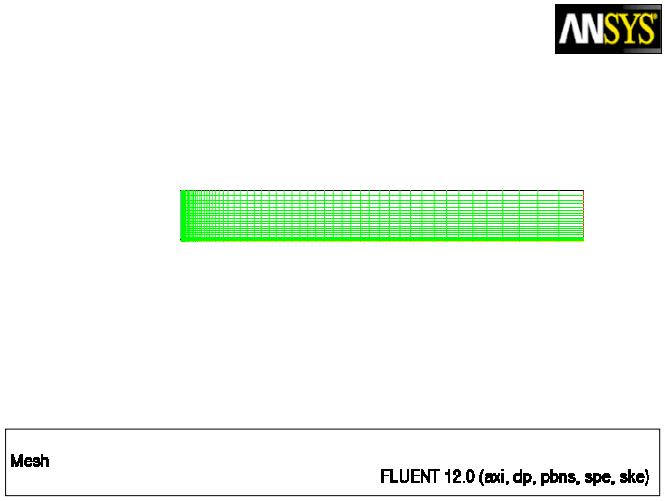
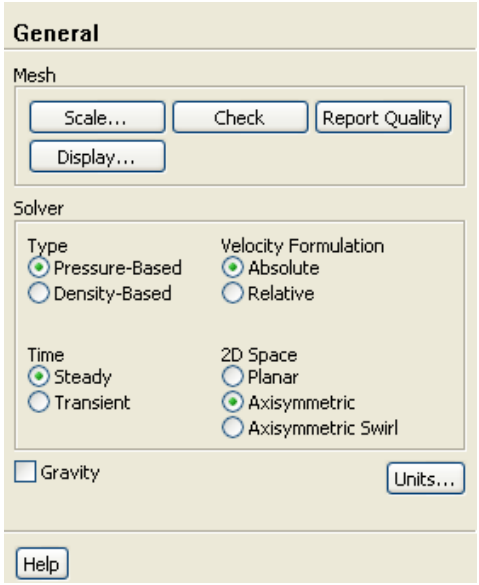


Figure 14.2: The Quadrilateral Mesh for the Combustor Model

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.

   General

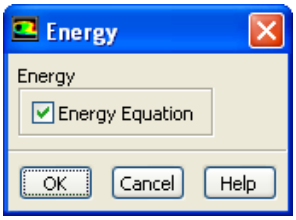


Step 3: Models

Models

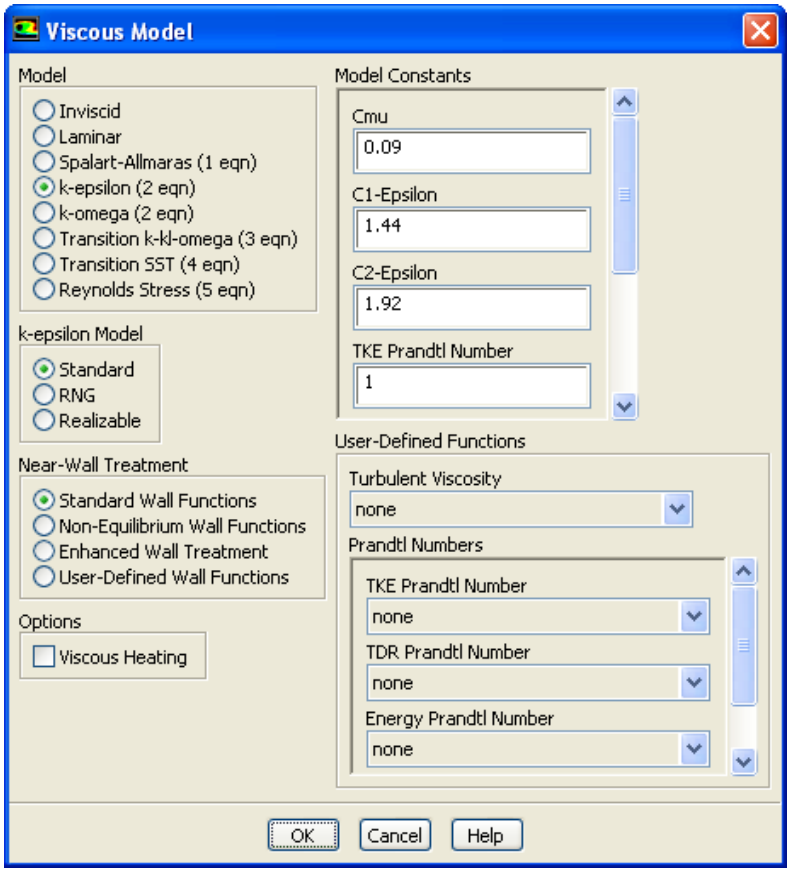
1. Enable heat transfer by enabling the energy equation.

   Models → Energy → Edit...



2. Select the standard k-ϵ turbulence model.

   Models → Viscous → Edit...



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

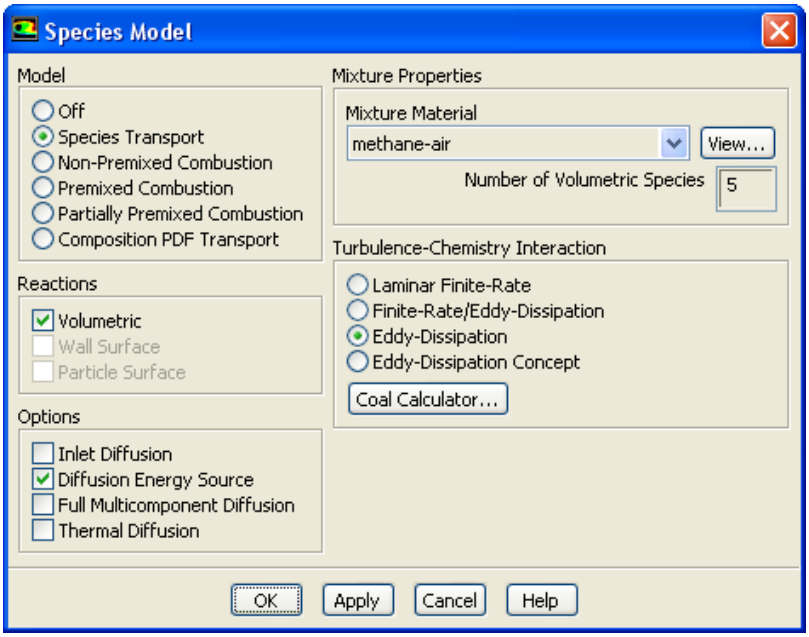
   The Viscous Model *dialog box will expand to provide further options for the* k-epsilon *model.*

(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.

Models → Species → Edit...



(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.

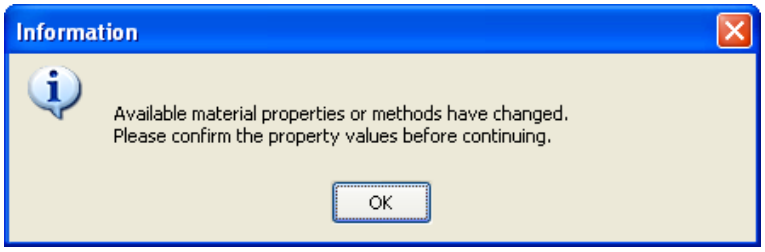
Note: *The* Mixture Material *list contains the set of chemical mixtures that exist in the* ANSYS FLUENT *database. You can select one of the pre-defined mixtures to access a complete description of the reacting system. The chemical species in the system and their physical and thermodynamic properties 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 Step 4: Materials).*

(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.

An Information *dialog box will open, reminding you to confirm the property values before continuing. Click* OK *to continue.*



ANSYS FLUENT *will display a warning about the symmetry zone in the console, prior to listing the properties that are required for the models you have enabled (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 Step 5: Boundary Conditions.

Step 4: Materials

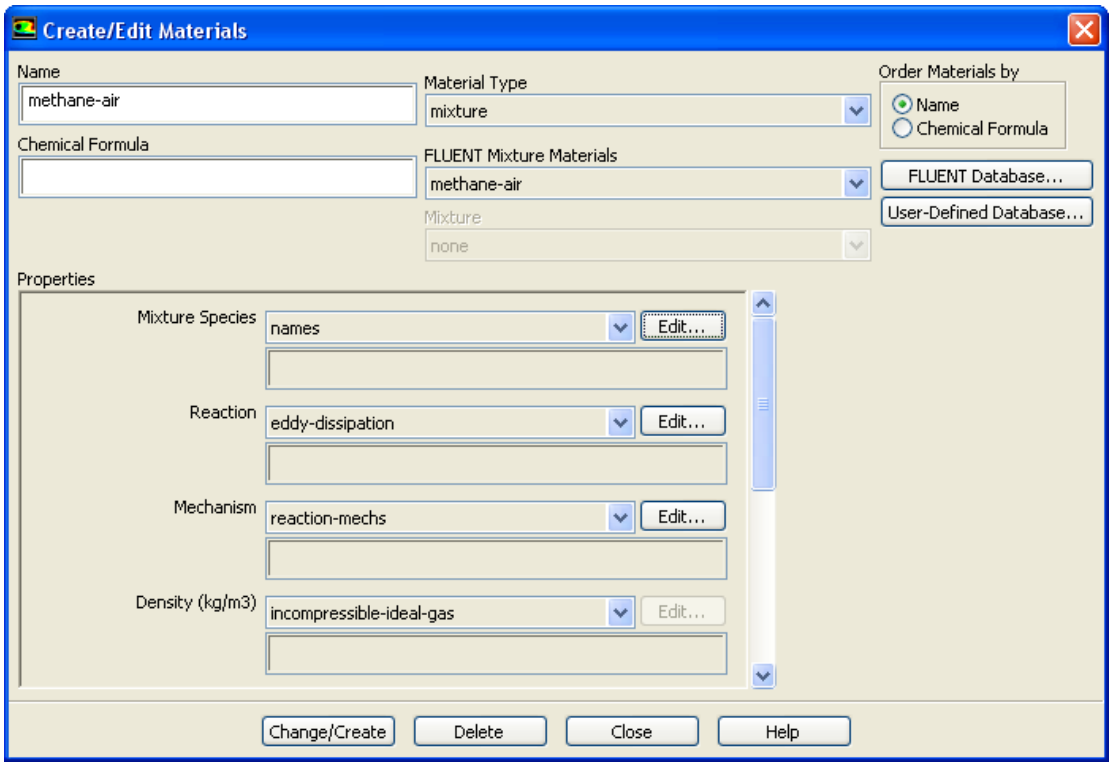
Materials

In this step, you will modify the default setting for the mixture by enabling the gas law. By default, the mixture material uses constant properties. Retain this constant property assumption for now, allowing only the mixture density to vary with temperature and composition. The influence of variable property inputs on the combustion prediction will be examined in a later part of the tutorial.

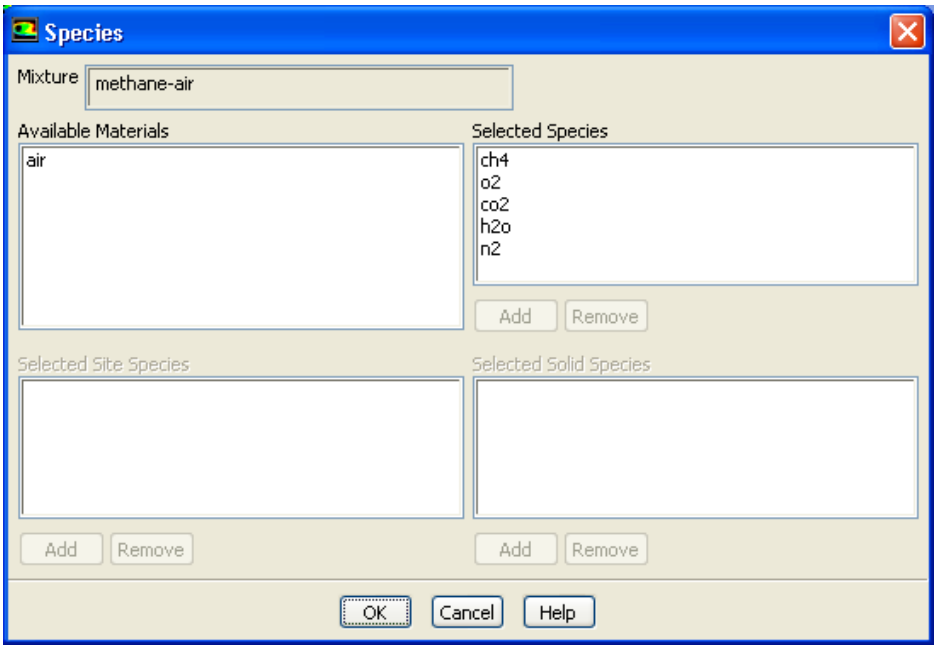
1. Revise the properties for the mixture materials.

   Materials → Mixture → Create/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* ANSYS 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.



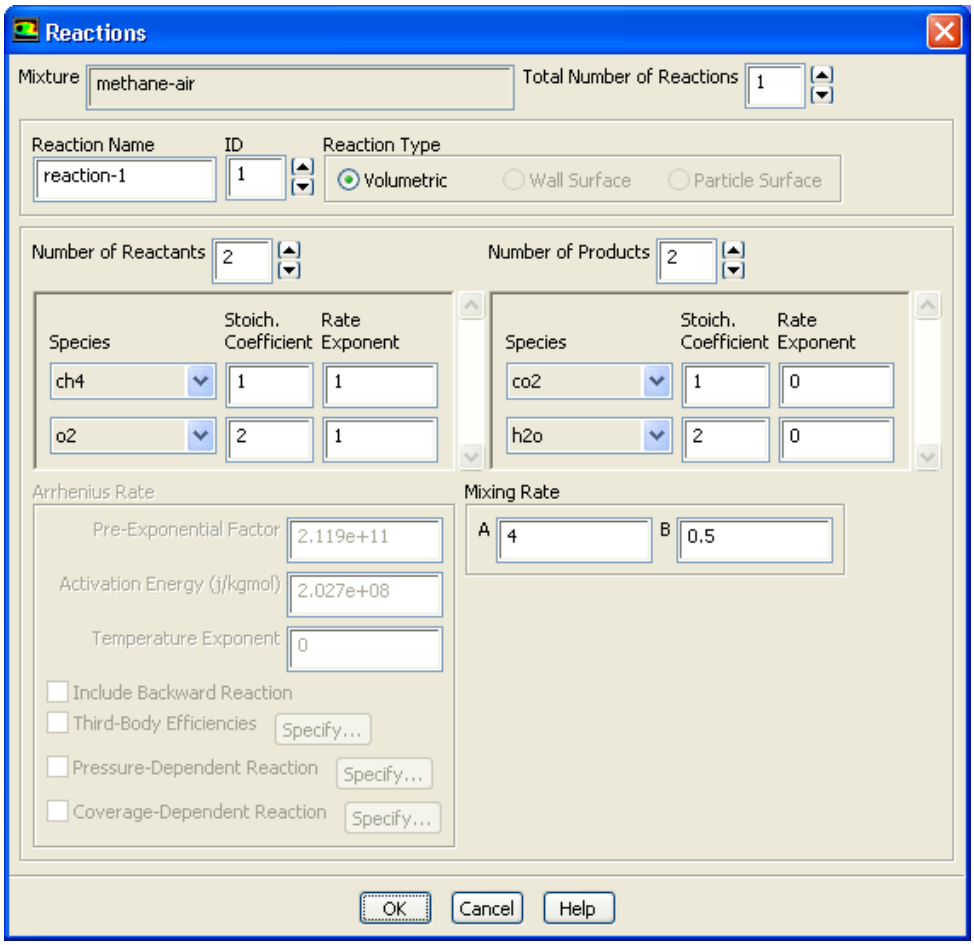
You can add or remove species from the mixture material as necessary using the Species *dialog box.*

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.

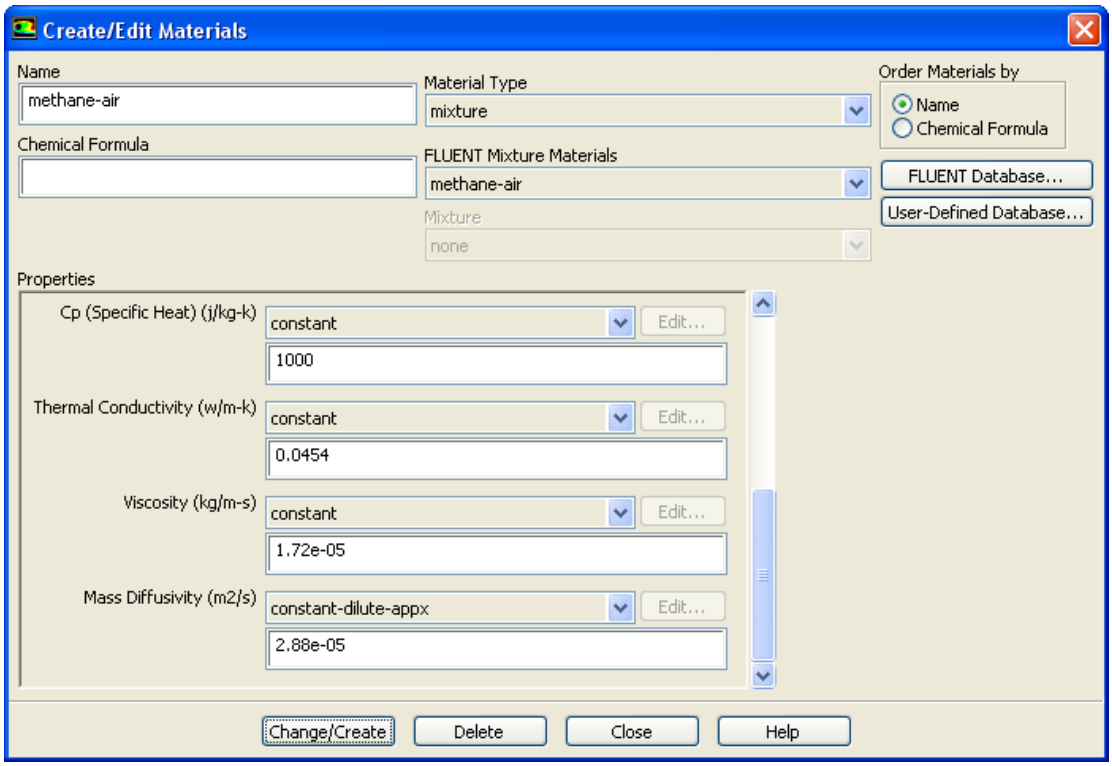


The eddy-dissipation reaction model ignores chemical kinetics (i.e., the Arrhenius rate) and uses only the parameters in the Mixing Rate *group box in the* Reactions *dialog box. The* Arrhenius Rate *group box will therefore be inactive. The values for* Rate Exponent *and* Arrhenius Rate *parameters 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) Select constant from the Cp drop-down list and enter 1000 J/kg − K for the specific heat value.

Scroll down to find the Cp *drop-down list and number-entry box.*

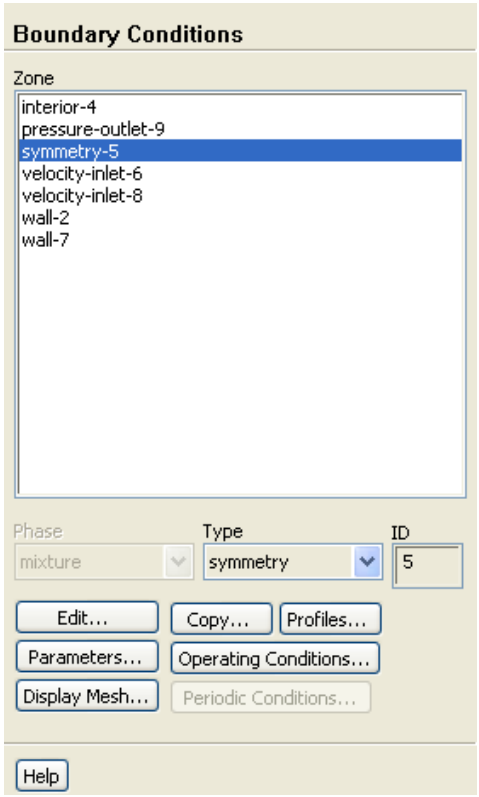
(e) Click Change/Create to accept the material property settings.

(f) Close the Create/Edit Materials dialog box.

The initial calculation will be performed assuming that all properties except density 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. The assumption of constant specific heat, however, has a strong effect on the combustion solution. You will change this property definition in Step 7: Solution with Varying Heat Capacity.

Step 5: Boundary Conditions

Boundary Conditions



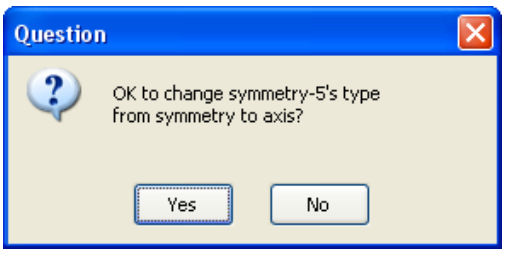
1. Convert the symmetry zone to the axis type.

   Boundary Conditions ⟶ symmetry-5

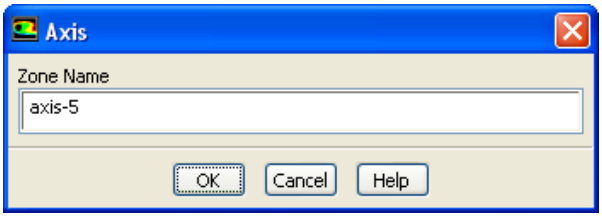
   The symmetry zone must be converted to an axis to prevent numerical difficulties where the radius reduces to zero.

   (a) Select axis from the Type drop-down list.

   A Question *dialog box will open, asking if it is OK to change the type of* symmetry-5 *from symmetry to axis. Click* Yes *to continue.*



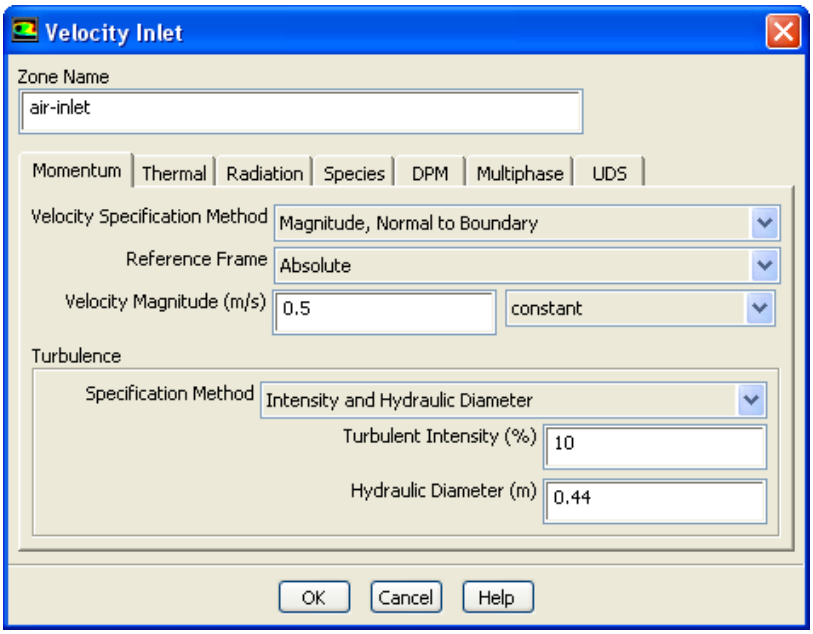
The Axis *dialog box will open and display the default name for the newly created axis zone. Click* OK *to continue.*



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

   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.

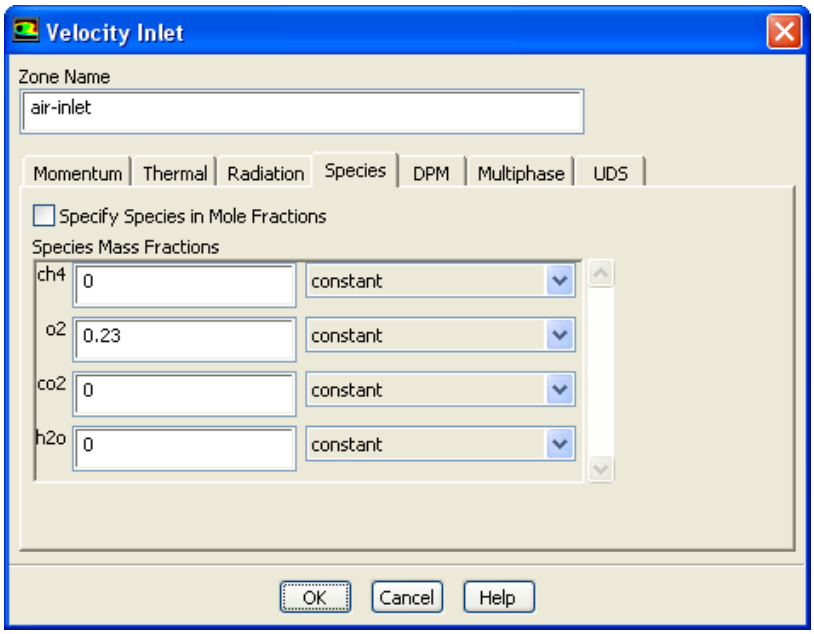
   (c) Select Intensity and Hydraulic Diameter from the Specification Method drop-down list in the Turbulence group box.

   (d) Retain the default value of 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.

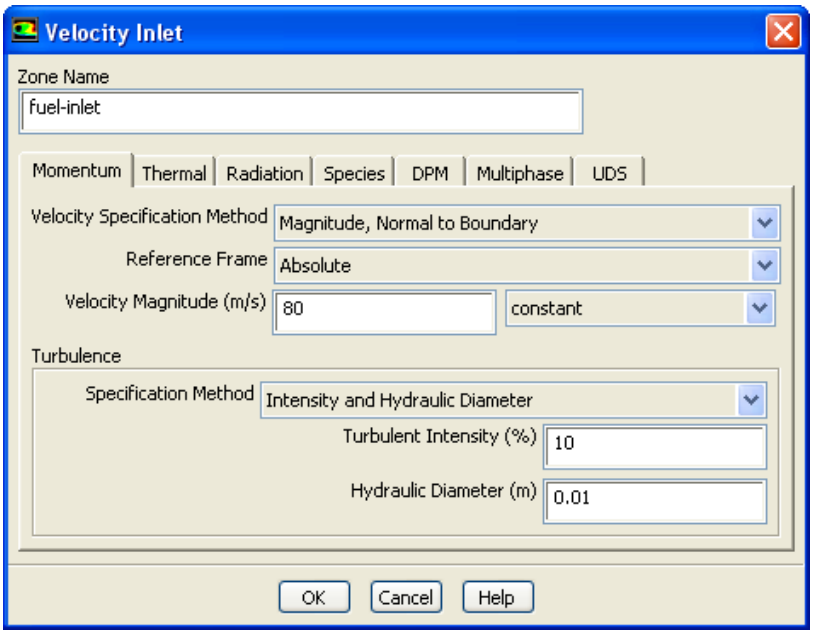
(g) Click the Species tab and enter `0.23` for o2 in the Species Mass Fractions group box.



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

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

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) Retain the default value of 10% for Turbulent Intensity.

(e) Enter 0.01 m for Hydraulic Diameter.

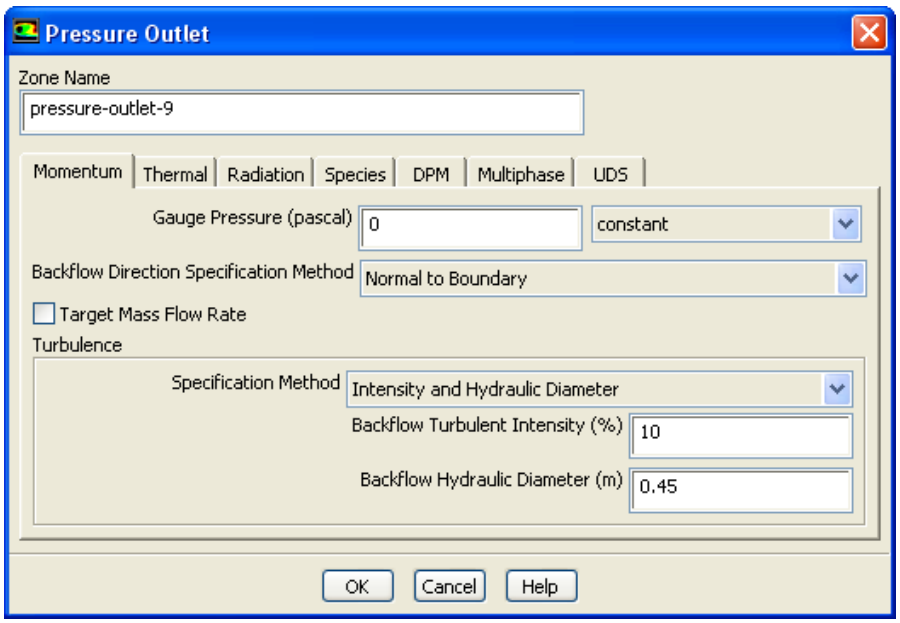
(f) Click the Thermal tab and retain the default value of 300 K for Temperature.

(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).

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) Retain the default value of 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.

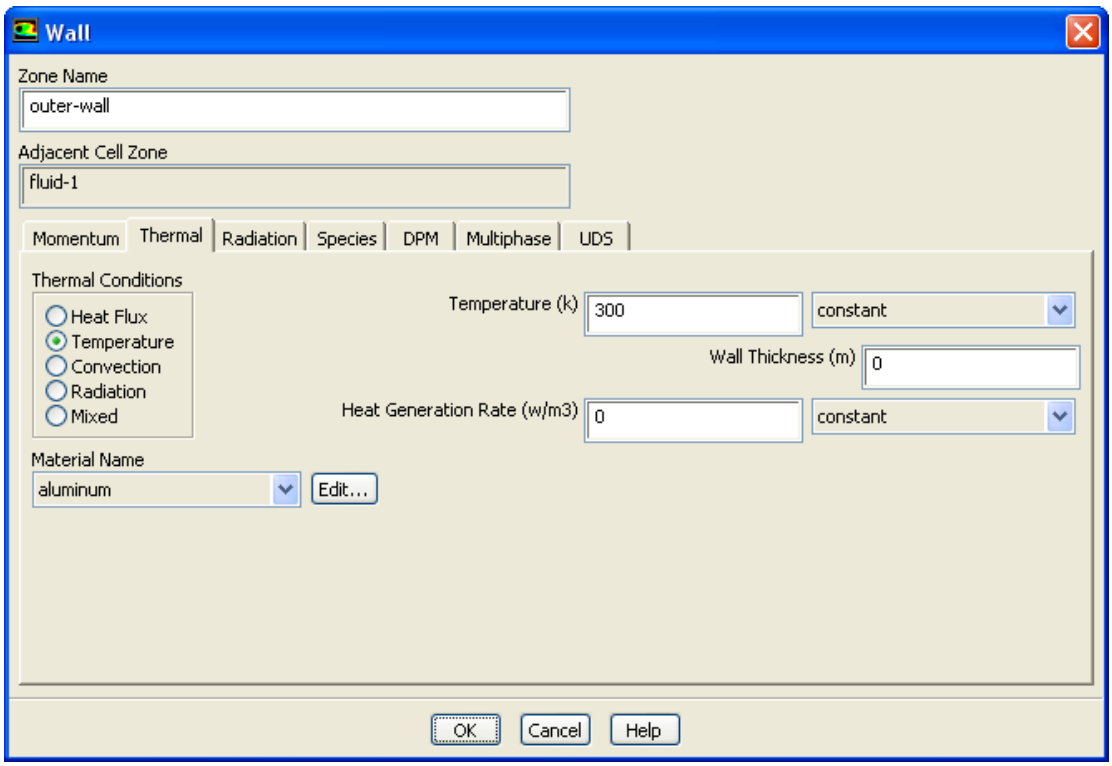
(g) Click OK to close the Pressure Outlet dialog box.

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).

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.

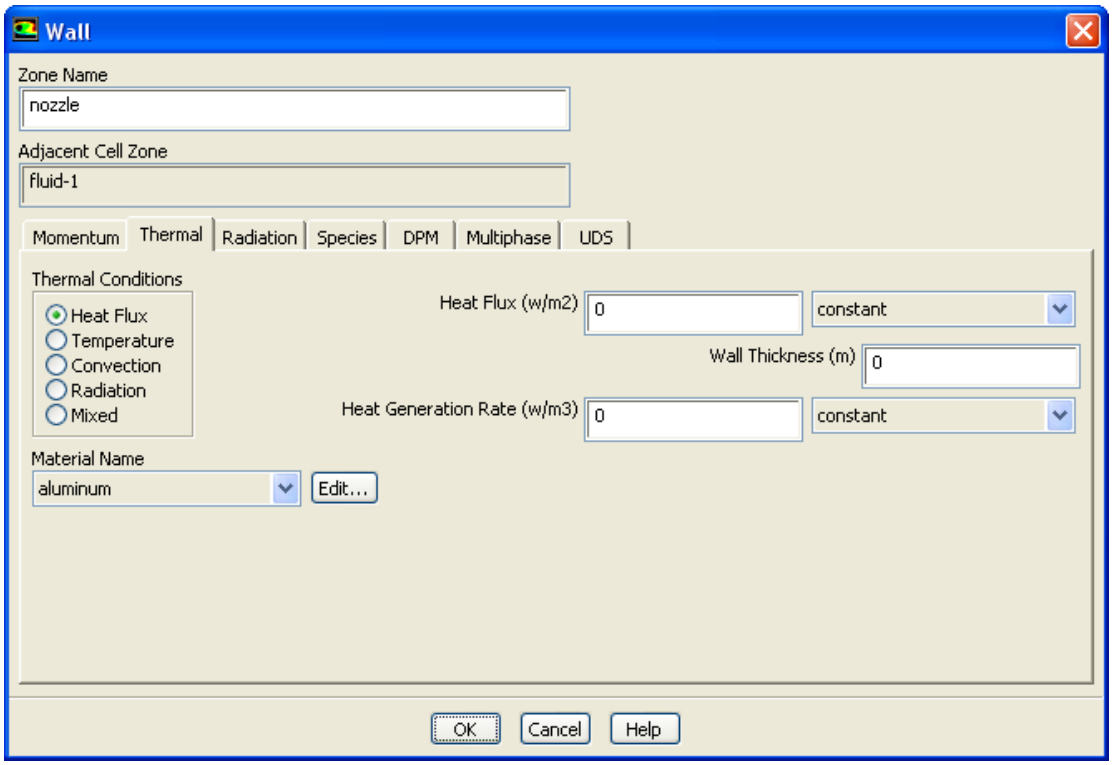
i. Select Temperature in the Thermal Conditions list.

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).

   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.

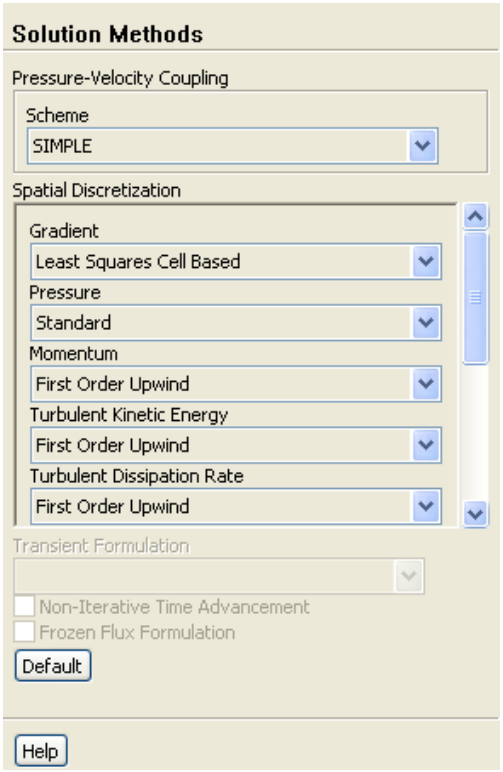
      ii. Retain the default value of `0` W/m^2 for Heat Flux, so that the wall is adiabatic.

   (c) Click OK to close the Wall dialog box.

Step 6: Initial Solution with Constant Heat Capacity

1. Retain the default solution parameters.

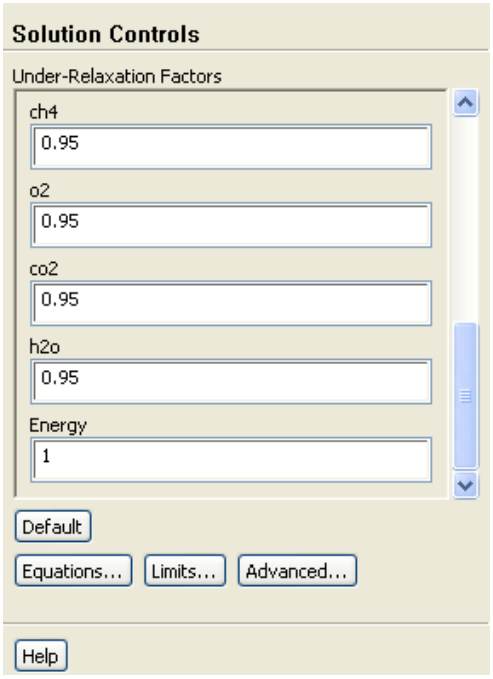
   Solution Methods



2. Set the under-relaxation factors for the species.

   Solution Controls

   The default under-relaxation parameters in ANSYS FLUENT *are set to high values. For a combustion model, it may be necessary to reduce the under-relaxation to stabilize the solution. Some experimentation is typically necessary to establish the optimal under-relaxation. For this tutorial, it is sufficient to reduce the species under-relaxation to 0.95.*

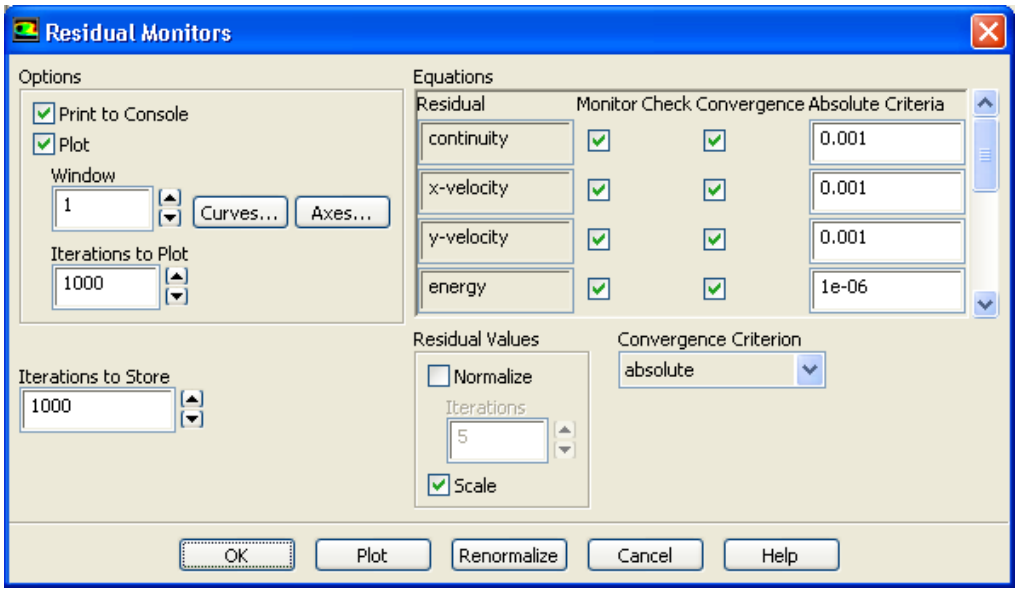


(a) Enter `0.95` for each of the species (ch4, o2, co2, and h2o) in the Under-Relaxation Factors group box.

Scroll down the Under-Relaxation Factors *group box to find the species.*

3. Ensure the plotting of residuals during the calculation.

Monitors → Residuals → Edit...

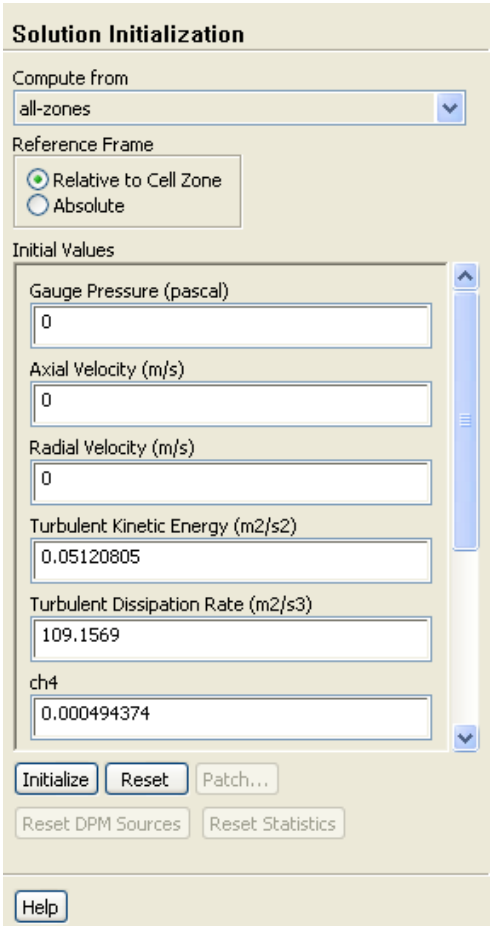


(a) Ensure that Plot is enabled in the Options group box.

(b) Click OK to close the Residual Monitors dialog box.

4. Initialize the field variables.

   Solution Initialization



   (a) Select all-zones from the Compute From drop-down list.

   (b) Click Initialize to initialize the variables.

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

   File ⟶ Write ⟶ Case...

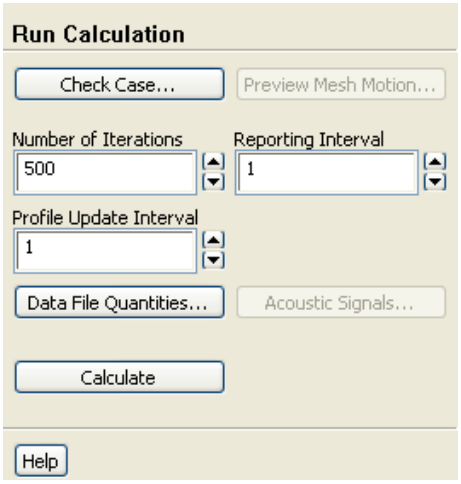
   (a) Enter `gascomb1.cas.gz` for Case File.

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

   (c) Click OK close the Select File dialog box.

6. Start the calculation by requesting 500 iterations.

   Run Calculation



   The solution will converge in approximately 280 iterations.

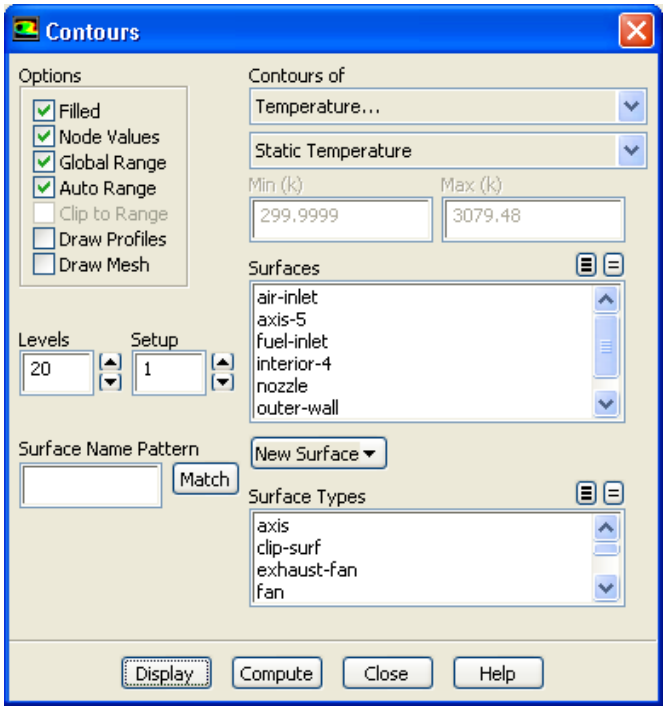
7. Save the case and data files (`gascomb1.cas.gz` and `gascomb1.dat.gz`).

   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.*

8. Review the current state of the solution by displaying filled contours of temperature.

   Graphics and Animations → Contours → Set Up...



   (a) Enable Filled in the Options group box.

   (b) Select Temperature... and Static Temperature from the Contours of drop-down lists.

   (c) Click Display (See Figure 14.3) and close the Contours dialog box.

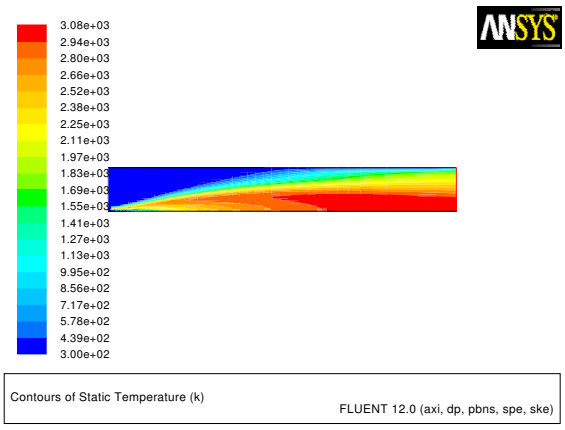


Figure 14.3: Contours of Temperature: Constant C_p

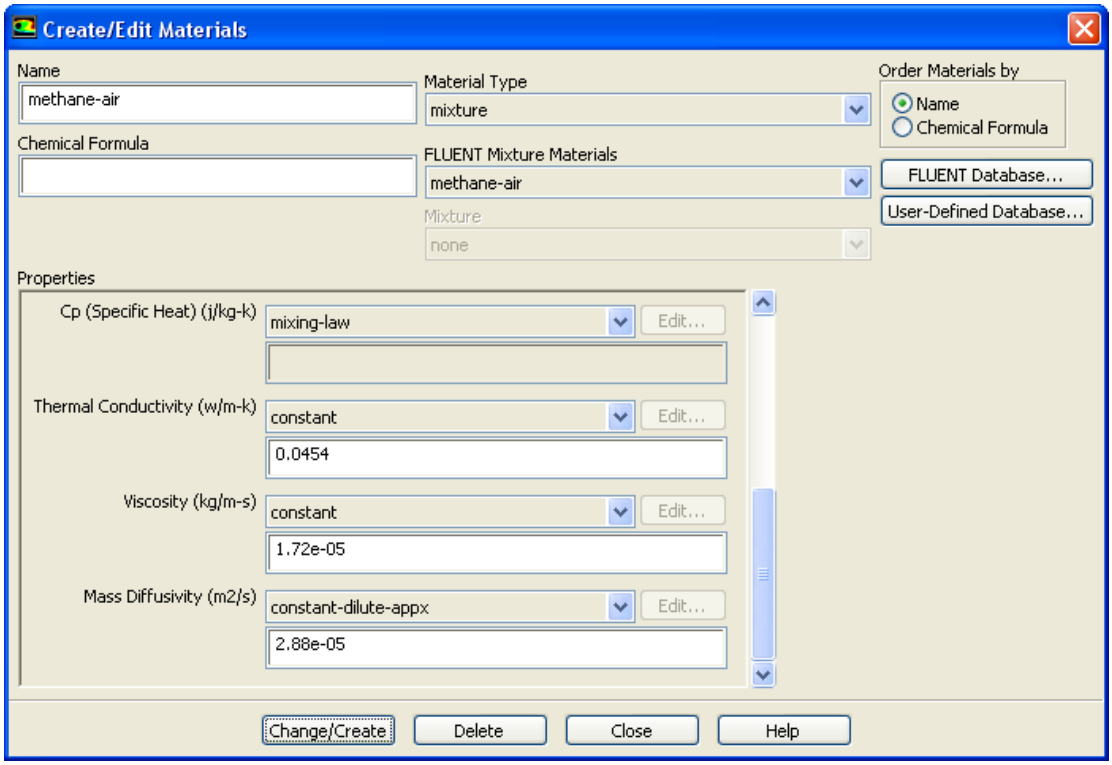
The peak temperature, predicted using a constant heat capacity of 1000 J/kg – K, is over 3000 K. This overprediction of the flame temperature can be remedied by a more realistic model for the temperature and composition dependence of the heat capacity, as illustrated in the next step of the tutorial.

Step 7: Solution with Varying Heat Capacity

The strong temperature and composition dependence of the specific heat has a significant impact on the predicted flame temperature. In this step you will use the temperature-varying property information in the ANSYS FLUENT *database to recompute the solution.*

1. Enable composition dependence of the specific heat.

   Materials ⟶ Mixture ⟶ Create/Edit...



   (a) Select mixing-law from the Cp drop-down list in the Properties group box.

   Scroll up the list to find mixing-law.

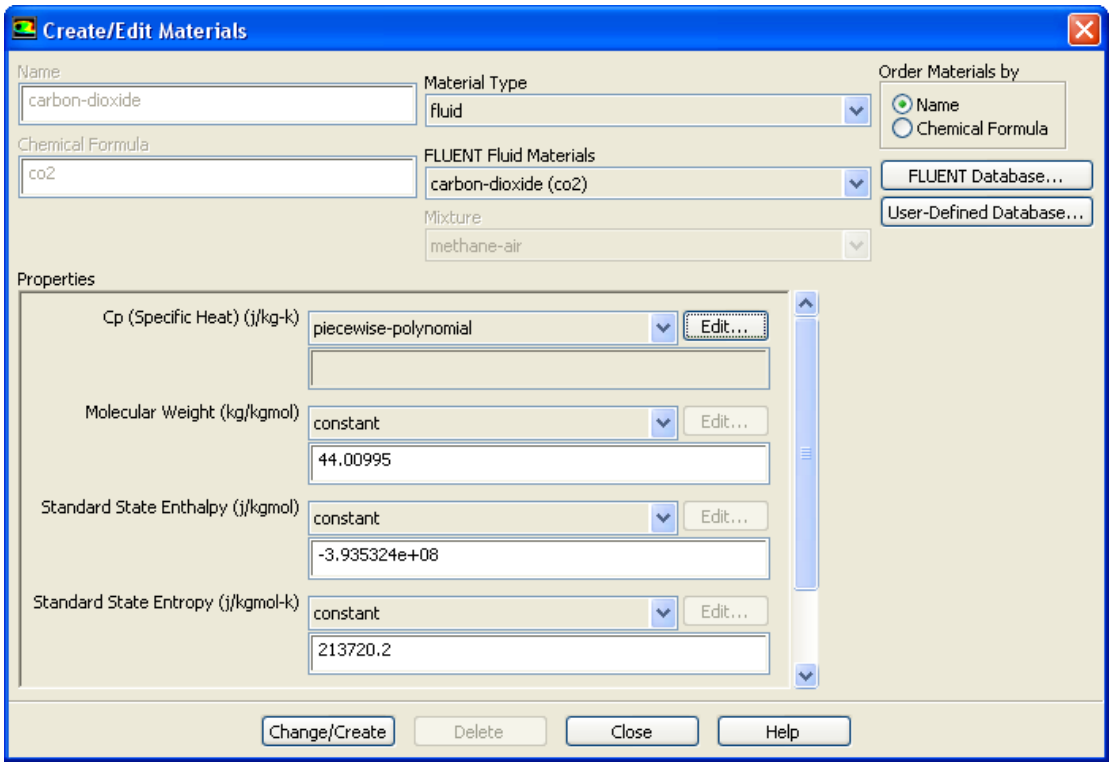
   (b) Click Change/Create.

   The specific heat of the mixture will now be based on a local mass-fraction-weighted average of all the species.

   (c) Close the Create/Edit Materials dialog box.

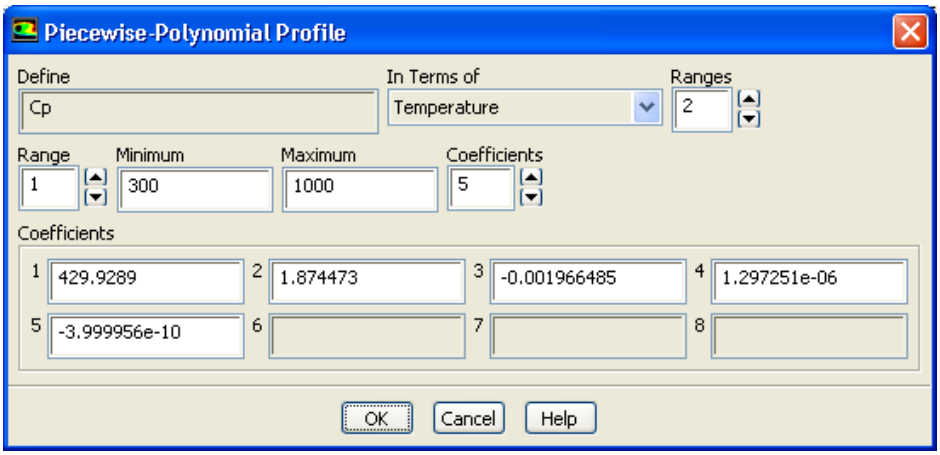
2. Enable temperature dependence of the specific heat for CO_2.

   Materials → carbon-dioxide → Create/Edit...



   (a) Ensure that piecewise-polynomial is selected from the Cp drop-down list in the Properties group box.

   (b) Click the Edit... button to open the Piecewise-Polynomial Profile dialog box.



      i. Retain the default values in the Coefficients group box.

      The default coefficients describe the polynomial $C_p(T)$ and are extracted from the ANSYS FLUENT *property database.*

ii. Click OK to close the Piecewise-Polynomial Profile dialog box.

(c) Close the Create/Edit Materials dialog box.

3. Similarly, ensure that temperature dependence of specific heat is enabled for the remaining species (CH_4, N_2, O_2, and H_2O).

4. Request 500 more iterations.

   Run Calculation

   The residuals will jump significantly as the solution adjusts to the new specific heat representation. The solution will converge after approximately 235 additional iterations.

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

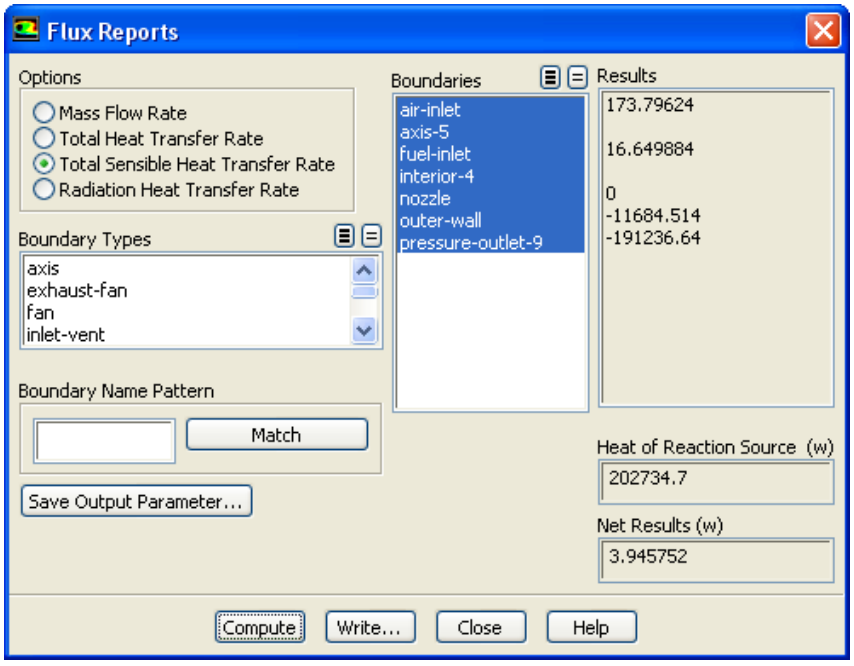
   File ⟶ Write ⟶ Case & Data...

Step 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.

   Reports ⟶ Fluxes ⟶ Set Up...



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

(b) Select all the boundaries from the Boundaries selection list.

(c) Click Compute and close the Flux Reports dialog box.

Note: *The energy balance is good. The net result is small compared to the heat reaction.*

2. Display filled contours of temperature (Figure 14.4).

Graphics and Animations → Contours → Set Up...

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

(b) Ensure that Temperature... and Static Temperature are selected in the Contours of drop-down lists.

(c) Click Display.

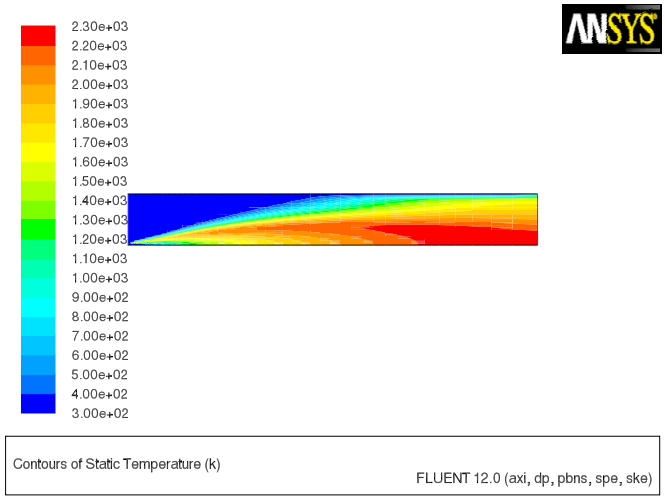


Figure 14.4: Contours of Temperature—Variable C_p

The peak temperature has dropped to approximately 2300 K *as a result of the temperature and composition-dependent specific heat.*

3. Display filled contours of specific heat (Figure 14.5).

Graphics and Animations → Contours → Set Up...

The contours of the mixture specific heat will show the variation of the specific heat within the domain.

(a) Select Properties... and Specific Heat (Cp) from the Contours of drop-down lists.

(b) Click Display and close the Contours dialog box.

The mixture specific heat is largest where the CH_4 is concentrated, near the fuel inlet, and where the temperature and combustion product concentrations are large. The increase in heat capacity, relative to the constant value used before, substantially lowers the peak flame temperature.

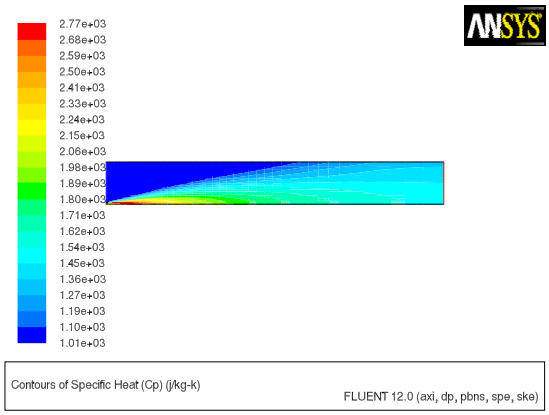
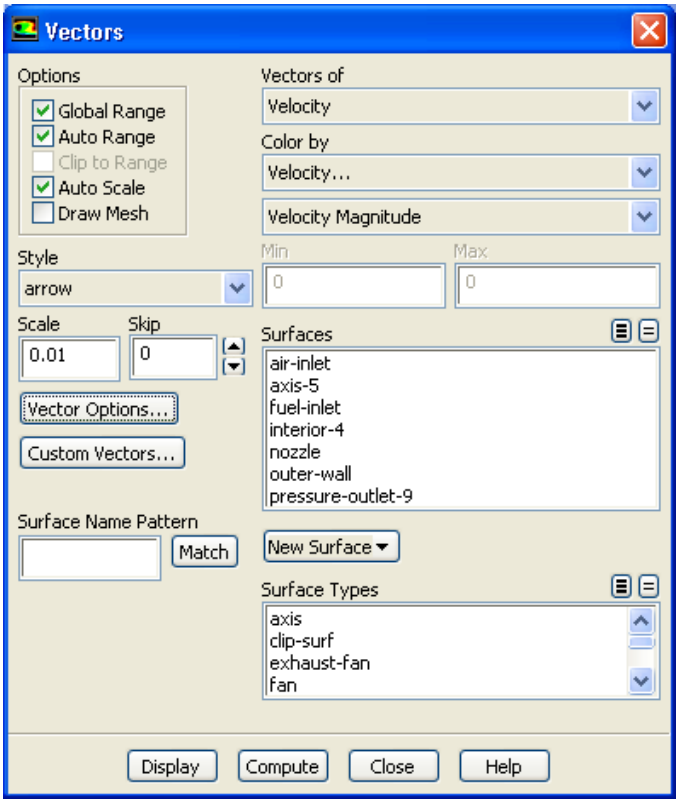


Figure 14.5: Contours of Specific Heat

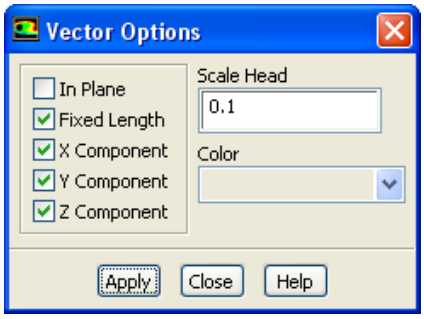
4. Display velocity vectors (Figure 14.6).

   Graphics and Animations → Vectors → Set Up...



(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.

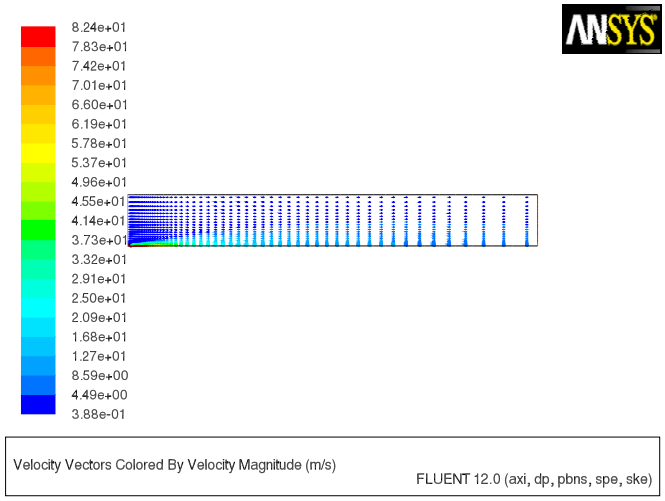


Figure 14.6: Velocity Vectors—Variable C_p

5. Display filled contours of stream function (Figure 14.7).

Graphics and Animations → Contours → Set Up...

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

(b) Click Display.

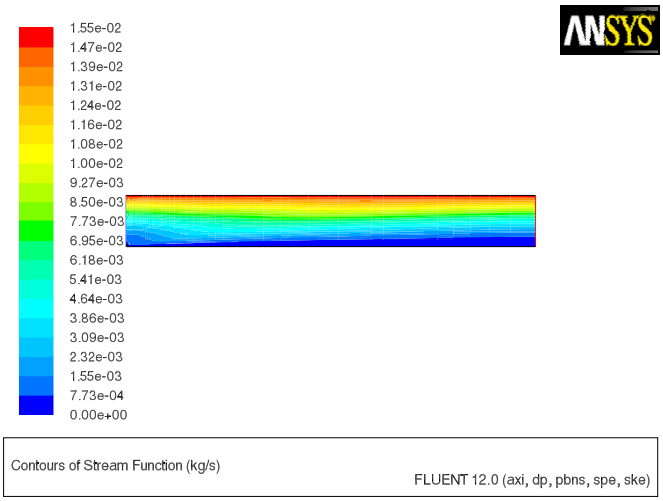


Figure 14.7: Contours of Stream Function—Variable C_p

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

6. Display filled contours of mass fraction for CH_4 (Figure 14.8).

   Graphics and Animations → Contours → Set Up...

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

   (b) Click Display.

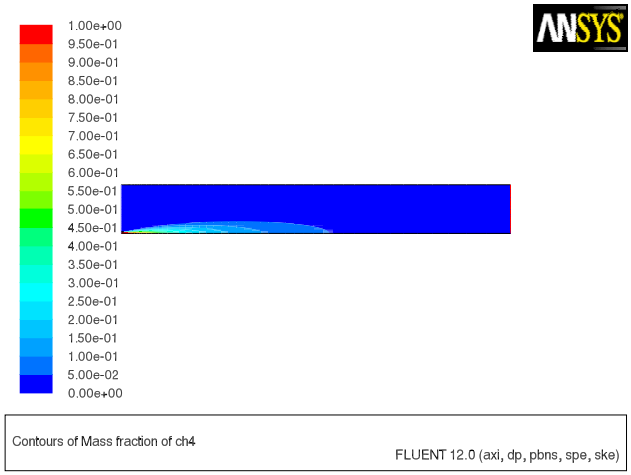


Figure 14.8: Contours of CH_4 Mass Fraction

7. In a similar manner, display the contours of mass fraction for the remaining species O_2, CO_2, and H_2O (Figures 14.9, 14.10, and 14.11). Close the Contours dialog box when all of the species have been displayed.

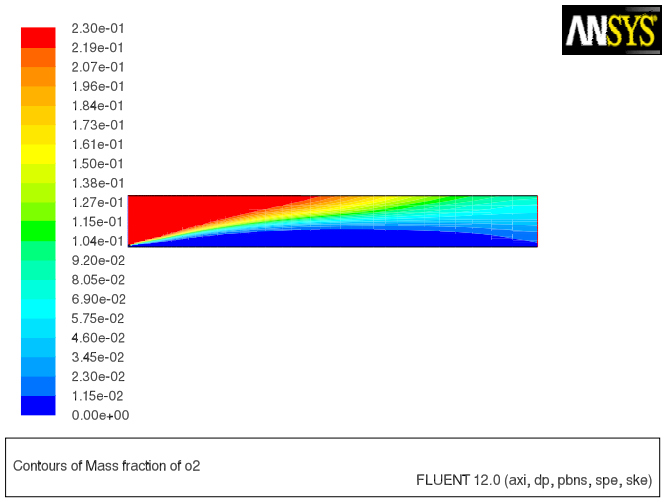


Figure 14.9: Contours of O_2 Mass Fraction

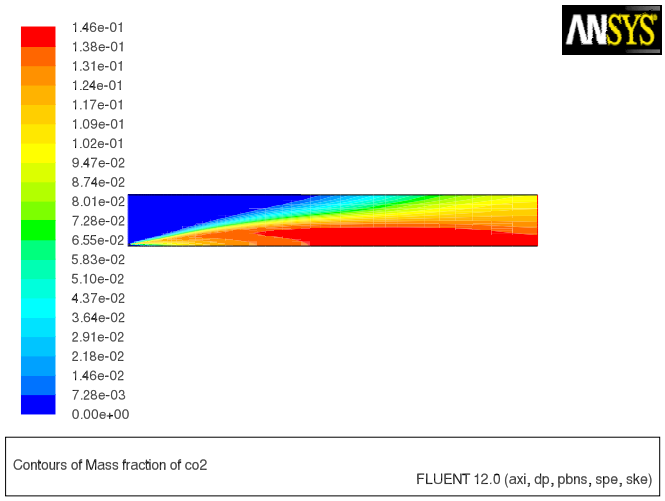


Figure 14.10: Contours of CO_2 Mass Fraction

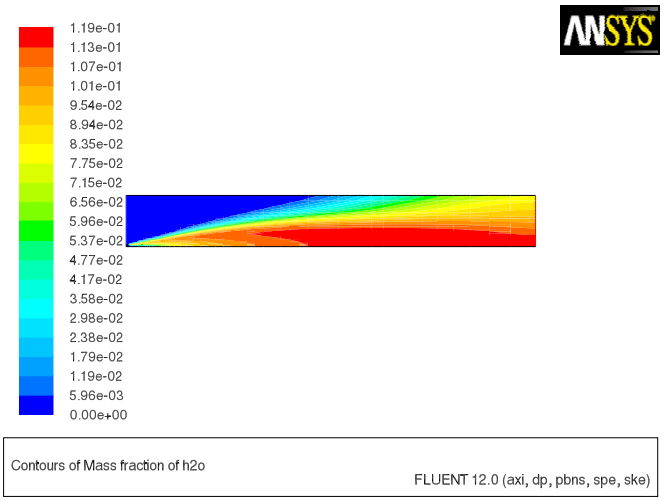
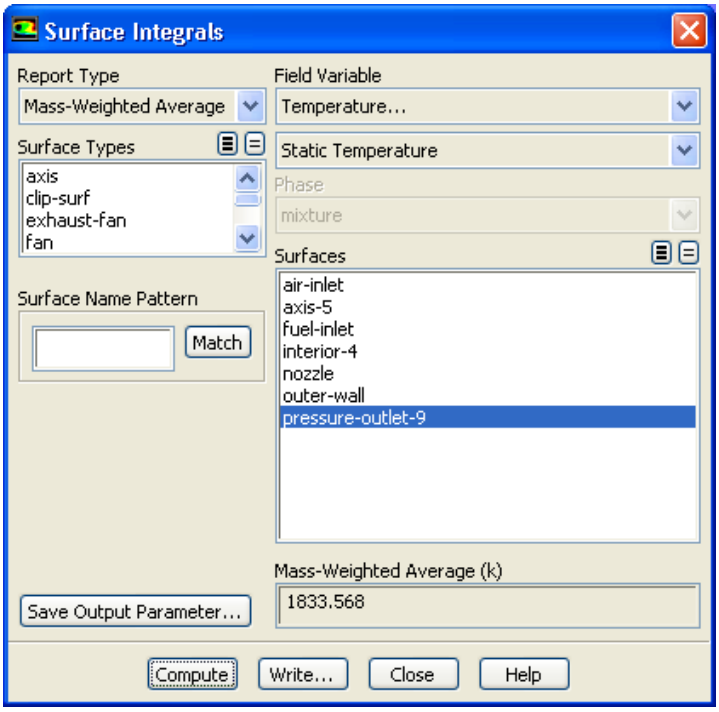


Figure 14.11: Contours of H_2O Mass Fraction

8. Determine the average exit temperature.

   Reports ⟶ Surface Integrals ⟶ Set Up...



   (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:

$$\overline{T} = \frac{\int T\rho\vec{v}\cdot d\vec{A}}{\int \rho\vec{v}\cdot d\vec{A}} \tag{14.2}$$

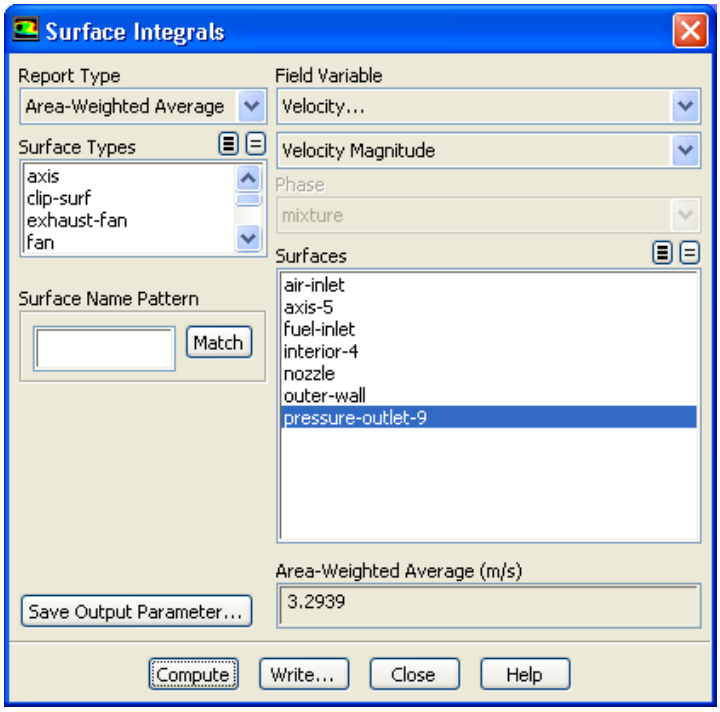
(c) Select pressure-outlet-9 from the Surfaces selection list, so that the integration is performed over this surface.

(d) Click Compute.

The Mass-Weighted Average *field will show that the exit temperature is approximately 1834* K.

9. Determine the average exit velocity.

Reports ⟶ Surface Integrals ⟶ Set Up...



(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:

$$\bar{v} = \frac{1}{A}\int v\, dA \tag{14.3}$$

(c) Click Compute.

The Area-Weighted Average *field will show that the exit velocity is approximately 3.29* m/s.

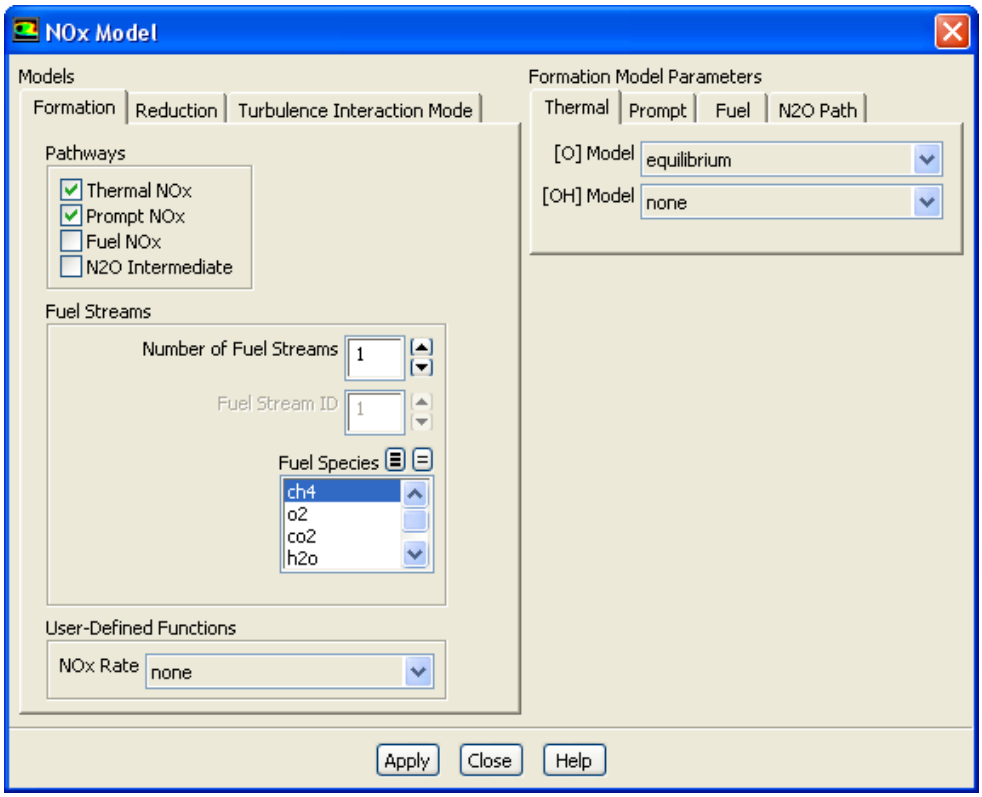
(d) Close the Surface Integrals dialog box.

Step 9: NO_x Prediction

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

1. Enable the NO_x model.

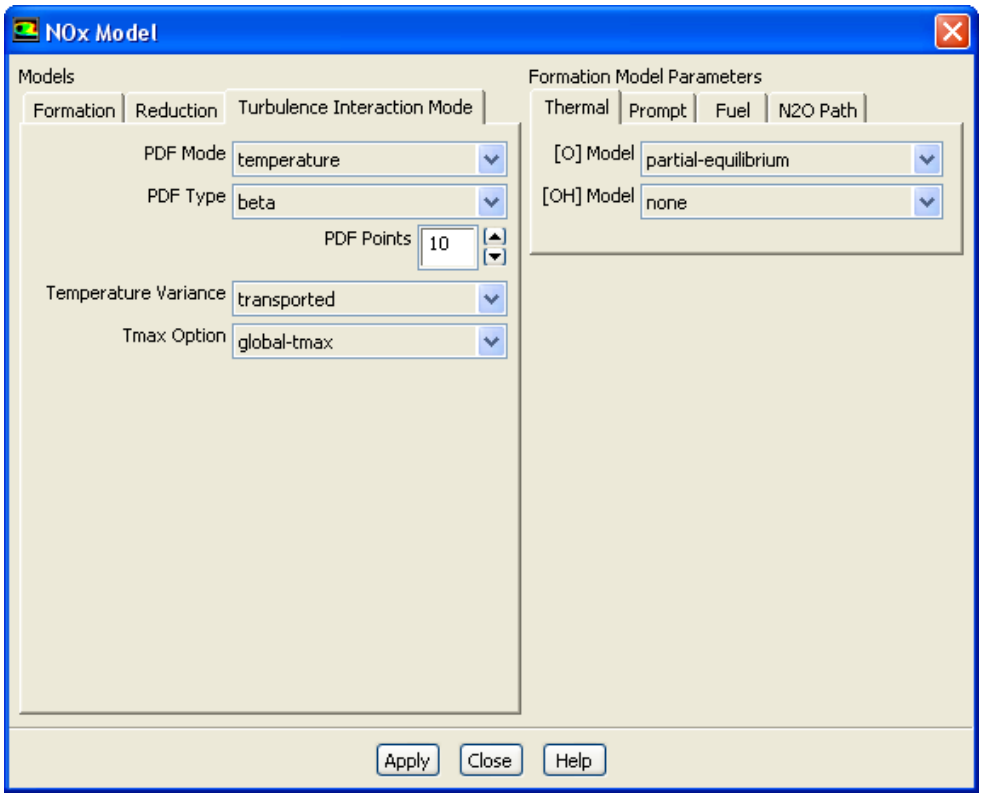
   Models → NOx → Edit...



(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 NO_x 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 the default value of 10 for PDF Points.

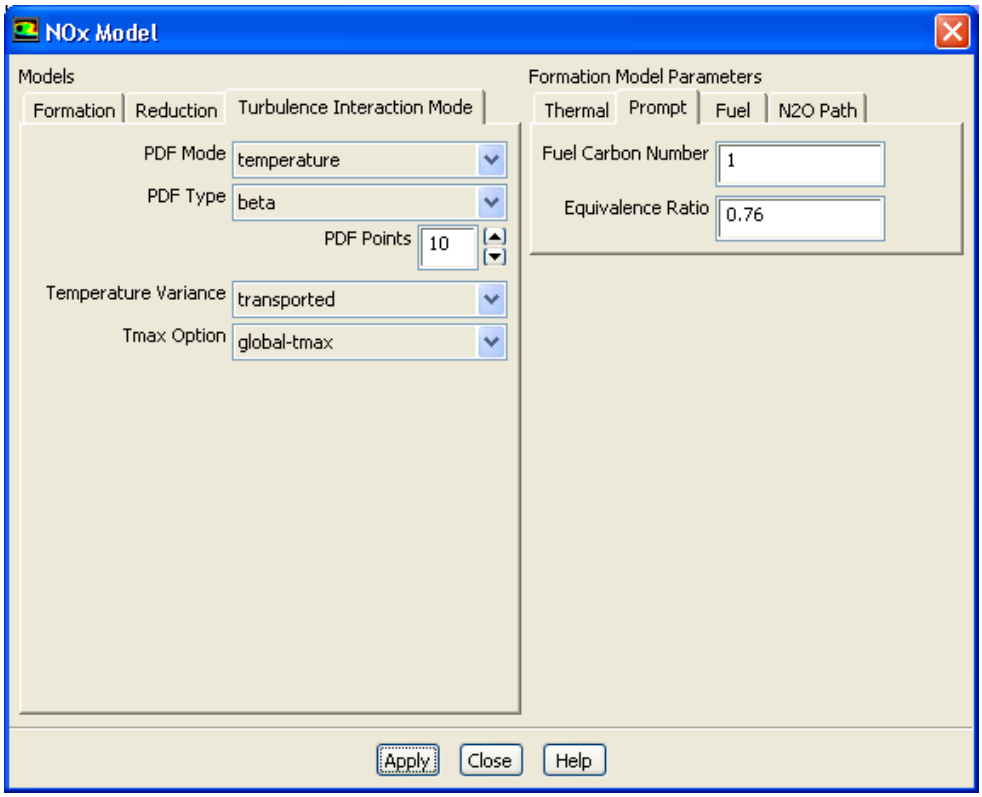
You can increase the value for PDF Points *to obtain a more accurate NO_x prediction.*

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 NO_x prediction.

(e) Click the Prompt tab.



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

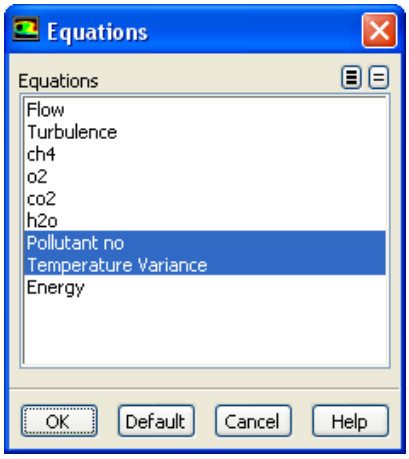
ii. Enter `0.76` for Equivalence Ratio.

All of the parameters in the Prompt *tab are used in the calculation of prompt NO_x 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.

   Solution Controls → Equations...

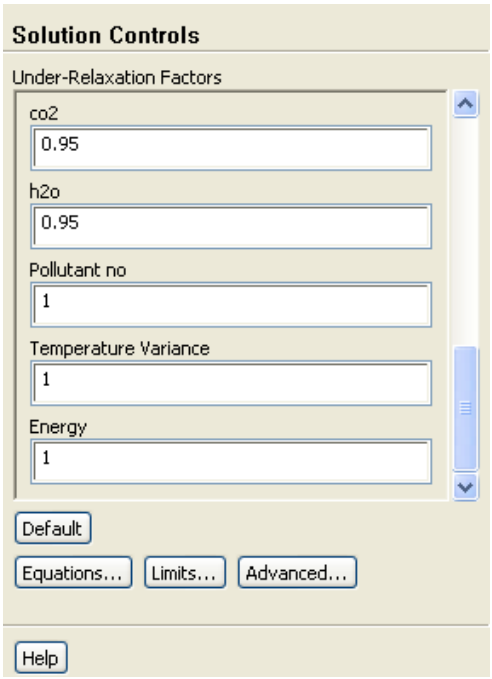


   (a) Deselect all variables except Pollutant no and Temperature Variance from the Equations selection list.

   (b) Click OK to close the Equations dialog box.

3. Set the under-relaxation factor for Pollutant no.

   Solution Controls

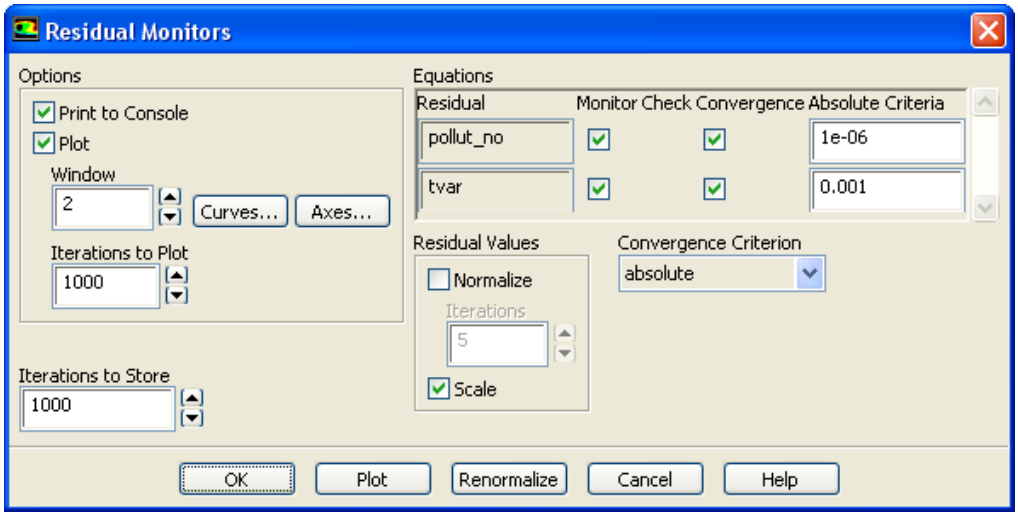


   (a) Enter 1 for Pollutant no and Temperature Variance in the Under-Relaxation Factors group box.

You will predict NO_x 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.

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

   Monitors ⟶ Residuals ⟶ Edit...



   (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 50 more iterations.

   Run Calculation

   The solution will converge in approximately 10 iterations.

6. Save the new case and data files (`gascomb3.cas.gz` and `gascomb3.dat.gz`).

   File ⟶ Write ⟶ Case & Data...

7. Review the solution by displaying contours of NO mass fraction (Figure 14.12).

   Graphics and Animations ⟶ Contours ⟶ Set Up...

   (a) Disable Filled in the Options group box.

   (b) Select NOx... and Mass fraction of Pollutant no from the Contours of drop-down lists.

   (c) Click Display and close the Contours dialog box.

   The peak concentration of NO is located in a region of high temperature where oxygen and nitrogen are available.

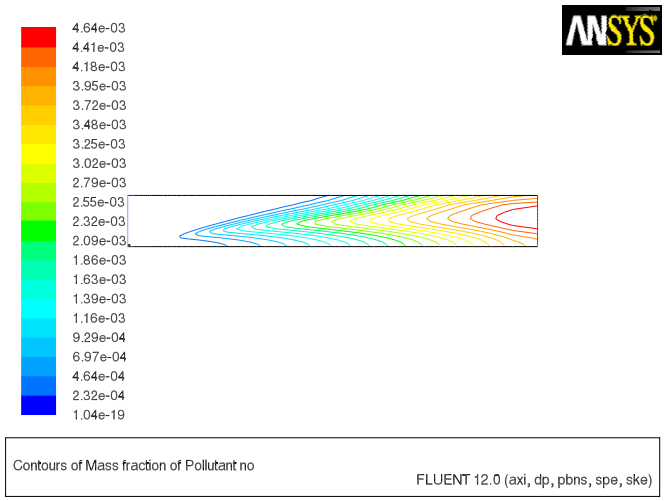
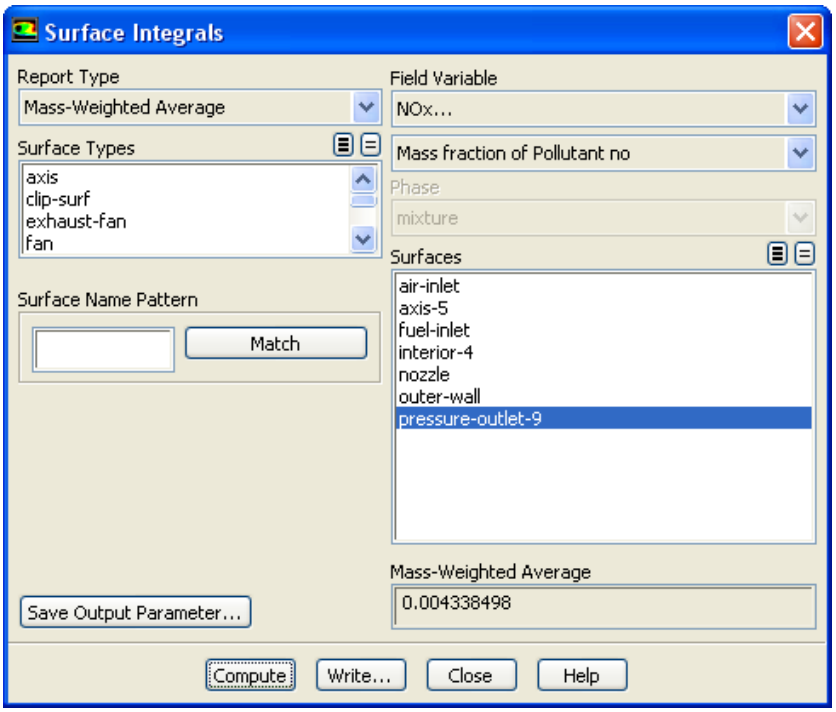


Figure 14.12: Contours of NO Mass Fraction—Prompt and Thermal NO_x Formation

8. Calculate the average exit NO mass fraction.

   Reports → Surface Integrals → Set Up...



   (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 0.0043.*

(e) Close the Surface Integrals dialog box.

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

Models ⟶ NOx ⟶ Edit...

(a) Click the Formation tab and disable Prompt NOx.

(b) Click Apply and close the NOx Model dialog box.

10. Request 50 iterations.

Run Calculation

The solution will converge in less than 10 iterations.

11. Review the thermal NO_x solution by viewing contours of NO mass fraction (Figure 14.13).

Graphics and Animations ⟶ Contours ⟶ Set Up...

(a) Ensure that NOx... and Mass fraction of Pollutant no are selected from the Contours of drop-down list.

(b) Click Display and close the Contours dialog box.

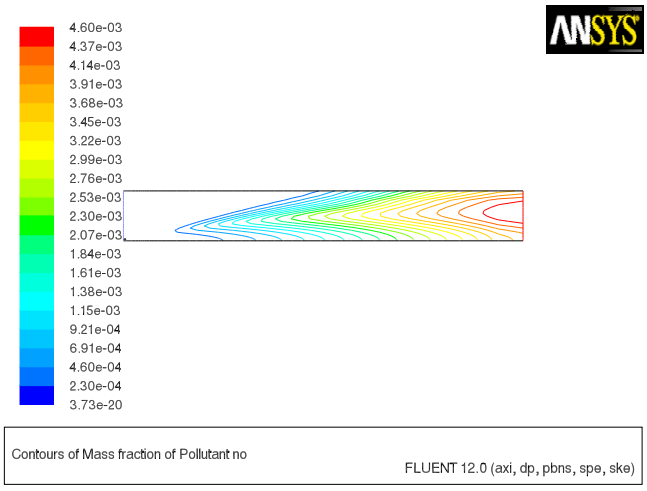


Figure 14.13: Contours of NO Mass Fraction—Thermal NO_x Formation

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

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

    Reports → Surface Integrals → Set Up...

    Hint: *Follow the same procedure you used earlier for the calculation with both thermal and prompt NO_x formation.*

    The Mass-Weighted Average *field will show that the exit NO mass fraction with only thermal NO_x formation (i.e., with no prompt NO_x formation) is approximately 0.0043.*

13. Solve for prompt NO_x production only.

    Models → 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 50 iterations.

    Run Calculation

    The solution will converge in less than 10 iterations.

15. Review the prompt NO_x solution by viewing contours of NO mass fraction (Figure 14.14).

    Graphics and Animations → Contours → Set Up...

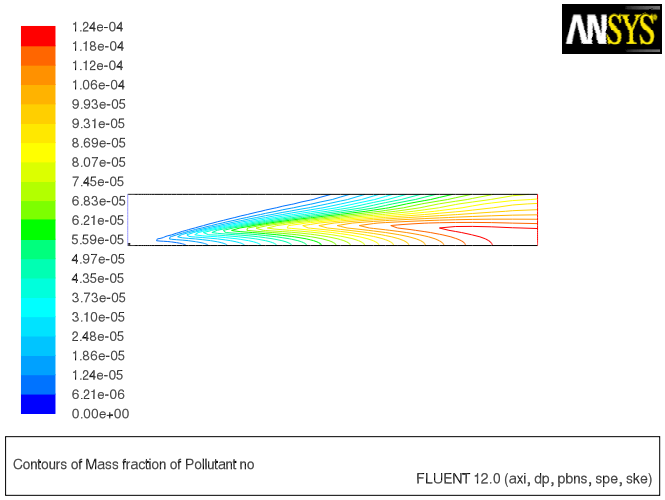


Figure 14.14: Contours of NO Mass Fraction—Prompt NO_x Formation

The prompt NO_x 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 with only prompt NO_x formation.

    Reports ⟶ Surface Integrals ⟶ Set Up...

    Hint: *Follow the same procedure you used earlier for the calculation with both thermal and prompt NO_x formation.*

    The Mass-Weighted Average *field will show that the exit NO mass fraction with only prompt NO_x formation is approximately 9.74633e-05.*

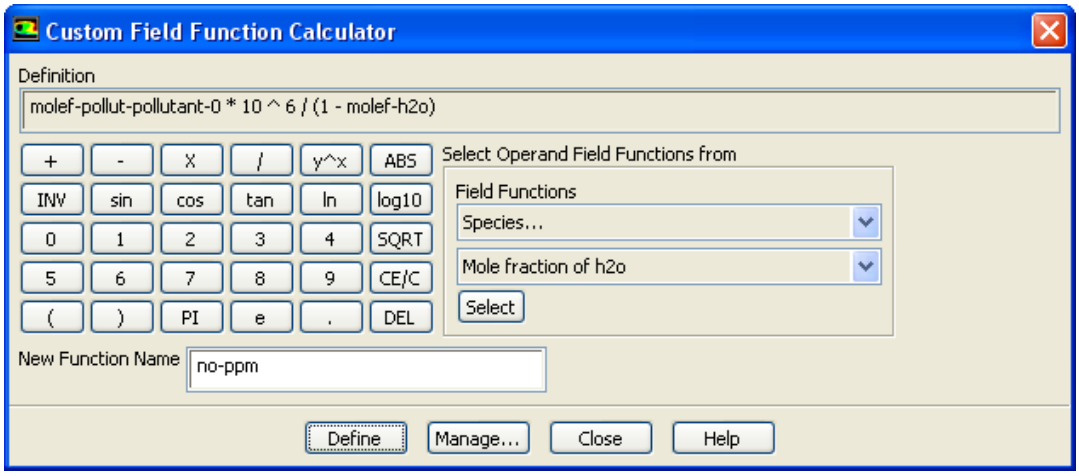
    Note: *The individual thermal and prompt NO mass fractions do not add up to the levels predicted with the two models combined. This is because reversible reactions are involved. NO produced in one reaction can be destroyed in another reaction.*

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

    NO ppm will be computed from the following equation:

$$\text{NO ppm} = \frac{\text{NO mole fraction} \times 10^6}{1 - \text{H}_2\text{O mole fraction}} \tag{14.4}$$

    Define ⟶Custom Field Functions...



    (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.

Hint: *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, For details Tutorial 1 .

(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 14.15).

Graphics and Animations → Contours → Set Up...

(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.

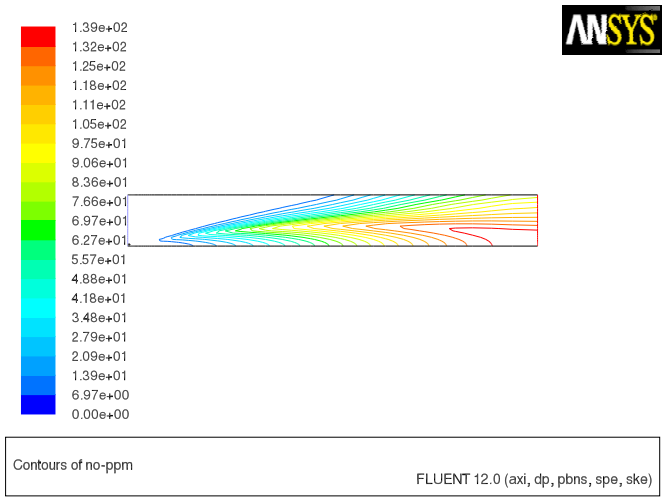


Figure 14.15: Contours of NO ppm—Prompt NO_x Formation

The contours closely resemble the mass fraction contours (Figure 14.14), as expected.

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 and modifying 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.

This exercise illustrated the important role of the mixture heat capacity in the prediction of flame temperature. The combustion modeling results are summarized in the following table.

	Peak Temp. (K)	Exit Temp. (K)	Exit Velocity (m/s)
Constant C_p	3080	2241	4.03
Variable C_p	2300	1834	3.29

Note: *Some of the values in the table were not explicitly calculated during the tutorial.*

The use of a constant C_p results in a significant overprediction of the peak temperature. The average exit temperature and velocity are also overpredicted.

The variable C_p solution produces dramatic improvements in the predicted results. Further improvements are possible by considering additional models and features available in ANSYS FLUENT, as discussed in the following section.

The NO_x 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.

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 Chapter 16 in the separate 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:

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

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 Section 13.3 in the separate 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 Tutorial 1.