Chapter 13: Modeling Species Transport and Gaseous Combustion

This tutorial is divided into the following sections:

13.1. Introduction
13.2. Prerequisites
13.3. Problem Description
13.4. Background
13.5. Setup and Solution
13.6. Summary
13.7. Further Improvements

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 .





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 $CH_4+2O_2 \rightarrow CO_2+2H_2O$ (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
13.5.2. Mesh
13.5.3. General Settings
13.5.4. Models
13.5.5. Materials
13.5.6. Boundary Conditions
13.5.7. Initial Reaction Solution
13.5.8. Postprocessing
13.5.9. NOx Prediction

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 \rightarrow Read \rightarrow 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 \rightarrow Mesh \rightarrow 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 \rightarrow Mesh \rightarrow Scale...

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

💶 Scale M	esh			X				
- Domain E	Extents			Scaling				
Xmin (m)	0	Xmax (m)	1.8	Onvert Units				
Ymin (m)	0	Ymax (m)	0.225	Specify Scaling Factors				
				Mesh Was Created In				
View Leng	th Unit In T			mm ▼ Scaling Factors X 0.001 Y 0.001 Scale Unscale				
	Close Help							

- 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 \rightarrow Mesh \rightarrow 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.



General	
Mesh	
Scale	Check Report Quality
Display	
Solver	
Type	Velocity Formulation
Pressure-Based	Absolute
O Density-Based	🔘 Relative
Time	2D Space
Steady	Planar
Transient	Axisymmetric
	Axisymmetric Swirl
Cravity	Units
Help	

13.5.4. Models

1. Enable heat transfer by enabling the energy equation.

```
Setting Up Physics \rightarrow Models \rightarrow Energy
 Setting Up Physics
                           User Defined
                                          Solving
                                                          Postprocessing
                                                                                Viewing
                                                                                           Parallel
                                                                                                     Design
                                                                                                              ∞
Solver
                                                                                  Models
Velocity Formulation
                   Operating Conditions...
                                                       Radiation ...
                                                                                 Multiphase...
                                                                                                         A Solidify/Melt...
 Absolute
                                            Energy Na Heat Exchanger...
                                                                                 Species...
                    Reference Values...
                                                                                                         D) Acoustics...
 Relative
                       Axisymmetric
                                                                                  Discrete Phase...
                                                                                                         H More
                                               Energy equation Jus...
```

2. Select the standard k- ε turbulence model.



Model	Model Constants			
🖱 Inviscid	Cmu			
🔘 Laminar	0.09			
Spalart-Allmaras (1 eqn)	C1-Epsilon			
k-epsilon (2 eqn)	1.44			
Transition k-kl-omena (3 eqn)	C2-Epsilon			
 Transition SST (4 eqn) 	1.92			
 Reynolds Stress (5 eqn) Scale-Adaptive Simulation (SAS) 	TKE Prandtl Number			
	1			
Detached Eddy Simulation (DES)	TDR Prandtl Number			
k-epsilon Model	1.3			
Near-Wall Treatment	Turbulent Viscosity			
Near-Wall Ireatment				
Scalable Wall Functions	Prandtl Numbers			
Non-Equilibrium Wall Functions	TKE Prandtl Number	^		
Enhanced Wall Treatment	(none			
Menter-Lechner	TDR Prandti Number			
User-Defined Wall Functions	(none	E		
Options	Energy Prandti Number			
Viscous Heating	None			
Production Kato-Launder				
	(none 👻			

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 \rightarrow Models \rightarrow Species...

Model	Mixture Properties Mixture Material
Species transport Non-Premixed Combustion	methane-air 👻 View
Premixed Combustion	Import CHEMKIN Mechanism
 Partially Premixed Combustion Composition PDF Transport 	Number of Volumetric Species 5
Reactions	Turbulence-Chemistry Interaction
Volumetric Volumetric Vall Surface Particle Surface Electrochemical	 Finite-Rate/No TCI Finite-Rate/Eddy-Dissipation Eddy-Dissipation Eddy-Dissipation Concept
Chemistry Solver	Coal Calculator
None - Explicit Source	
Options	
Inlet Diffusion	Select Boundary Species
 Diffusion Energy Source Full Multicomponent Diffusion Thermal Diffusion 	Select Monitored 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.

FSetup \rightarrow Materials \rightarrow Mixture \rightarrow methane-air $\stackrel{\bigcirc}{\Box}$ 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.

	22707242207		Order Heberich hu
Name	Material Type		Order Materials by
methane-air	mixture	•	Name
Chemical Formula	Fluent Mixture Materials		Chemical Formula
	methane-air	•	Guest Database
	Mixture		Filleric Database
	none	*	User-Defined Database
Properties			
Reaction eddy-diss Mechanism reaction- Density (kg/m3) ncompre	mechs ▼ Edit) Edit		

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

Mixture methane-air	
Available Materials	Selected Species
air	ch4 o2 co2 h2o n2 Add Remove
Selected Site Species	Selected Solid Species
Add Remove	Add Remove
	OK Cancel Help

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.

ir		Total Nu	mber of Reactions	1	
ID Re	action Type				
1 💿 🔍	Volumetric 🔘 \	Wall Surface 🔘 Part	ticle Surface 🔘 Elec	trochemical	
nts 2 🌩		Number of Prod	ucts 2 🜩		
Stoich. Coefficient	Rate Exponent	Species	Stoich. Coefficient	Rate Exponent	
• 1	1	E co2	•]1	0	1
▼ 2	1	h2o	▼]2	0	1
		Mixing Rate			
ntial Factor 2.119	8+11	A 4	B 0.5		
(j/kgmol) 2.027	e+08				
Exponent 0					
vard Reaction	Specify				
ficiencies	Specify				
endent Reaction	Specify				
endent Reaction	Specify				
	ir ID Re 1 Stoich. Coefficient 1 2 Stoich. Coefficient 1 2 Stoich. Coefficient 2 Stoich. Coefficient 2 Stoich. Coefficient 2 Stoich. Coefficient 2 Stoich. Coefficient 2 Stoich. Coefficient 2 Stoich. Coefficient 2 Stoich. Coefficient 2 Stoich. Coefficient 2 Stoich. Coefficient 2 Stoich. Coefficient 2 Stoich. Coefficient 2 Stoich. Coefficient 2 Stoich. Coefficient 2 Stoich. Coefficient 2 Stoich. Coefficient 2 Stoich. Coefficient 2 Stoich. Stoich. Coefficient 2 Stoich. Stoich. Coefficient 2 Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich. Stoich	ir ID Reaction Type Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumetric Volumet	Total Nu ID Reaction Type 1 • Volumetric Wall Surface Part nts 2 • Number of Prod Stoich. Coefficient Exponent • 1 1 1 1 • 2 1 1 • 2 1 1 • 1 • 2 • Mixing Rate A 4 Mixing Rate A 4	ir Total Number of Reactions	ir Total Number of Reactions 1 ID Reaction Type 1 • Volumetric Wall Surface Particle Surface Electrochemical Ints 2 • Number of Products 2 • Stoich. Rate Exponent 1 1 1 • 2 1 1 • 2 0 • Mixing Rate A 4 B 0.5 Mixing Rate A 4 B 0.5

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.

ame		Material Type				Order Materials by
methane-air		mixture			•	Name
Chemical Formula	F	Fluent Mixture Materia	ls			Chemical Formula
		methane-air			*	Fluent Database
	1	Mixture				User-Defined Database
		none			*	Osci Denned Database
roperties						
Cp (Specific Heat) (j/kg-k)	nixing-law		• Edit	<u>^</u>		
Thermal Conductivity (w/m-k)	constant		▼ Edit.,.			
i i	0.0454					
Viscosity (kg/m-s)	constant		▼ Edit			
1	.72e-05					
Mass Diffusivity (m2/s)	constant-dilute-appx		• Edit			
2	.88e-05					
				-		

- 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

Boundary Conditions
Zone Filter Text
interior-4
pressure-outlet-9
symmetry-5
velocity-inlet-6
velocity-inlet-8
wall-2
waii-7
Phase Type ID
Edit Copy Profiles
Parameters
Display Mesh
Periodic Conditions
Help
() Cip

1. Convert the symmetry zone to the axis type.

Setup \rightarrow **Conditions** $\rightarrow \stackrel{\frown}{=}$ 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).



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.

Velocity Inlet								×	
Zone Name									
air-inlet									
Momentum	Thermal	Radiation	Species	DPM	Mul	tiphase	Potential	UDS	
Velocity Specification Method Magnitude, Normal to Boundary									
Reference Frame Absolute									
	Velocity Magnitude (m/s) 0.5								
Supersonic/Init	Supersonic/Initial Gauge Pressure (pascal) 0								
	- Turbulence	9							
	Specificatio	n Method Int	tensity and I	Hydraulic	Diame	ter			
Turbulent Intensity (%) 10							P		
Hydraulic Diameter (m) .44								P	
	OK Cancel Help								

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 **Tur-bulence** 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.

💶 Velocity	Inlet					×
Zone Name	9					
air-inlet						
Momentu	um Thermal	Radiation Species	DPM	Multiphase	Potential	UDS
	Specify Spec	ies in Mole Fractions				
Species M	ass Fractions					
ch4	0	constant		•		
o2	0.23	constant		•		
co2	0	constant		•		
h2o	0	constant		•		
		OK Canc	Help			

- h. Click **OK** to close the **Velocity Inlet** dialog box.
- 3. Set the boundary conditions for the fuel inlet (velocity-inlet-6).

Setup \rightarrow Boundary Conditions \rightarrow velocity-inlet-6	₫́ Edit
------------------------------------------------------------------------	---------

💶 Velocity Inlet								×
Zone Name								
fuel-inlet								
Momentum	Thermal	Radiation	Species	DPM	Mul	tiphase	Potential	UDS
Velocit	y Specificatio	on Method Ma	agnitude, N	ormal to I	Bound	lary		•
	Refere	nce Frame Ab	osolute					•
	Velocity Ma	gnitude (m/s)	80			cons	tant	•
Supersonic/Init	ial Gauge Pre	ssure (pascal)	0			cons	tant	•
	- Turbulence	9						
	Specification	n Method Int	ensity and H	Hydraulic	Diame	eter		-
			Turbulent I	Intensity	(%)	10		P
			Hydraulic	Diameter	(m)	0.01		P
		OK	Cancel	Help				

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).

Example : Setup \rightarrow Boundary Conditions \rightarrow pressure-outlet-9 $\stackrel{\bigcirc}{\rightarrow}$ Edit...

Pressure Out	let	×
Zone Name		
pressure-outlet	-9	
Momentum	Thermal Radiation Species DPM Multi	phase Potential UDS
В	ackflow Reference Frame Absolute	•
	Gauge Pressure (pascal) 0	constant 🔹
Backflow Direc	tion Specification Method Normal to Boundary	•
Backfl	ow Pressure Specification Total Pressure	•
🗐 Average Pr	essure Specification	
🔲 Target Mass	Flow Rate	
	Turbulence	
	Specification Method Intensity and Hydraulic Diam	eter 🔹
	Backflow Turbulent Intensity (%)	10 P
	Backflow Hydraulic Diameter (m)	0.45 P
	OK Cancel Help	

- 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**).

E Setup \rightarrow Boundary Conditions \rightarrow wall-7 $\stackrel{0}{\hookrightarrow}$ Edit...

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

Wall Wall										×
one warne outer-wall										
djacent Cell Zo luid-1	ne									
Momentum	Thermal	Radiation	Species	DPM	Mu	itophase	UDS	Wall Fi	im Potential	
Thermal Condit	tions									
🔿 Heat Flux			т	emperatu	re (k)	300			constant	•
Temperation	ure					Wall	Thickness	(m) 0		P
Convection Heat Generation Rate (w/m3			/m3)	0			constant	-		
 via System via Mappe 	n Coupling d Interface									
Material Name aluminum		Edit								
11										
			-	_						
			L	OK Can	cel	Help				

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).

E Setup \rightarrow Boundary Conditions \rightarrow wall-2 $\stackrel{\square}{\hookrightarrow}$ Edit...

ne Name ozzle Ijacent Cell Zo vid-1	ne										
Momentum	Thermal	Radiation	Species	DPM	Mu	tophase	UDS	Wall	Film	Potential	
hermal Condi Heat Flux	tions		He	eat Flux (w,	/m2)	0			const	tant	•
Convectio Radiation Mixed via Syster via Mappe	n Coupling d Interface	He	at Generatio	on Rate (w)	/m3)	Wall	Thickness	(m) 0	const	tant	Ţ
4aterial Name aluminum	•	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.



Solution Methods	
Pressure-Velocity Coupling	
Scheme	
Coupled 👻	
Spatial Discretization	_
Gradient	1
Least Squares Cell Based 🔻	
Pressure	-
Second Order 👻	=
Momentum	
Second Order Upwind 🔻	
Turbulent Kinetic Energy	
First Order Upwind 🔻	
Turbulent Dissipation Rate	
First Order Upwind 🔻	
Transient Formulation	
Non-Iterative Time Advancement	
Frozen Flux Formulation	
Pseudo Transient	
Warped-Face Gradient Correction	
High Order Term Relaxation Options	
Set All Species Discretizations Together	
Default	
Help	

- 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 \rightarrow Controls \rightarrow Controls...

Solution Controls	
Pseudo Transient Explicit Relaxation Factors	_
Pressure	-
0.5	
Momentum	Ε
0.5	
Density	-
0.25	
Body Forces	
1	
Turbulent Kinetic Energy	
0.75	
Turkulant Dissigntion Data	*
Default	
Equations Limits Advanced	
Set All Species URFs Together	

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.

Multigrid	Multi-S	Stage	Expert	
Spatial Discretization Limiter	÷8			
imiter Type				
Standard 🔹 🔻	l i			
 Cell to Face Limiting Cell to Cell Limiting Apply Limiter Filter 				
eudo Transient Method Usa	ge			_
	On/Of	f Under-Relaxat	ion Factor Time Scale Factor	
Turbulent Kinetic Ener	gy 🔽	0.8	1	
Turbulent Dissipation Ra	te 📝	0.8	1	
c	h4 🔽	1	10]
	02 🔽	1	10	
c	02 🔽	1	10	5
h	20 🔽	1	10	8
Ener	gy 🔽	1	10	5
Default				

- 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 \rightarrow Reports \rightarrow Residuals...

Print to Console Plot	Residual	Monit	or Check Convergence	e Absolute Criteria	
7 Plot				e ribbolace criceria	
	continuity			0.001	E
Window	x-velocity	V		0.001	Ļ
1 Curves Axes	y-velocity			0.001	
Iterations to Plot	energy			1e-06	
1000	Residual Values	Tital .	Co	nvergence Criterion	
erations to Store	🔲 Normalize		Iterations at	osolute	
000	Scale		<u> </u>	onvergence Conditio	ns
	Compute Loc	al Scale			

- 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

	Initializa	ition	
Method		Patch	
O Hybrid	More Settings	Reset Statistics	
Standard	Options	Reset DPM	t = 0 Initialize

- a. Retain the default **Hybrid** initialization method and click **Initialize** to initialize the variables.
- 5. Save the case file (gascomb1.cas.gz).

```
File \rightarrow Write \rightarrow 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 \rightarrow Run Calculation \rightarrow Advanced...
```

Run Calculation	
Check Case	Update Dynamic Mesh
Pseudo Transient Option Fluid Time Scale	DNS
 Time Step Method User Specified Automatic 	Timescale Factor 5
Length Scale Method	Verbosity
	0
Aggressive	
Number of Iterations 200 -	Reporting Interval
Number of Iterations 200 🗣 Profile Update Interval 1	Reporting Interval
Number of Iterations 200 Profile Update Interval 1 Data File Quantities	Reporting Interval 1
Number of Iterations 200 - Profile Update Interval 1 - Data File Quantities Calculate	Reporting Interval 1

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 \rightarrow Write \rightarrow 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.

Options Mass Flow Rate	Boundaries Filter Text	Results	
 Total Heat Transfer Rate Total Sensible Heat Transfer Rate Radiation Heat Transfer Rate 	air-inlet axis-5 fuel-inlet interior-4 nozzle outer-wall pressure-outlet-9	173.7963996081019 16.64988560719532 -0 -11787.92355890429 -192029.9785504543	
		4	
Save Output Parameter		Heat of Reaction Source (w)	
		203633.3	
		Net Results (w)	
		5.823312	

Postprocessing \rightarrow Reports \rightarrow 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 (1997)).
- 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 \rightarrow Graphics \rightarrow Contours \rightarrow 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.





The peak temperature is approximately 2310 K.

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

Postprocessing \rightarrow Graphics \rightarrow Vectors \rightarrow Edit...

Option	IS	Vectors of	Vectors of						
Global Range Auto Range Clip to Range		Velocity	Velocity Color by Velocity						
		Color by							
		Velocity							
Aut Drop	o Scale	Velocity Magnitu	Velocity Magnitude						
	W Mesn	Min (m/s)	Max (m/s)						
Style		0.4037463	82.27368						
Scale	Skip	Surfaces Filter 1	ext 🐻	.					
0.01 Vector Custom	0 Options I Vectors	air-inlet axis-5 fuel-inlet interior-4 nozzle outer-wall	Ĵ	E					
		Display Comp	ute Close Help						

- a. Enter 0.01 for Scale.
- b. Click the Vector Options... button to open the Vector Options dialog box.

Vector Options	×
🔲 In Plane	Scale Head
🗹 Fixed Length	0.1
X Component	
Y Component	
Z Component	
	Color
Apply	Close Help

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 \rightarrow Graphics \rightarrow Contours \rightarrow 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 CH₄ (Figure 13.6: Contours of CH4 Mass Fraction (p. 565)).

Postprocessing \rightarrow Graphics \rightarrow Contours \rightarrow 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 O₂, CO₂, and H₂O (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 \rightarrow Reports \rightarrow Surface Integrals...

Surface Integrals	
Report Type	Field Variable
Mass-Weighted Average	Temperature 🔹
Custom Vectors	Static Temperature 🗸
Vectors of	Surfaces Filter Text
Custom Vectors	air-inlet
	axis-5
Save Output Parameter	fuel-inlet
	interior-4
	nozzle
	outer-wall
	pressure-outlet-9
	Mass-Weighted Average (k)
	1839.818
Compute	rite Close Help

- 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:

$$\overline{T} = \frac{\int T\rho \vec{v} \cdot d\vec{A}}{\int \rho \vec{v} \cdot d\vec{A}}$$
(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 \rightarrow Reports \rightarrow Surface Integrals...

Surface Integrals	
Report Type	Field Variable
Area-Weighted Average 🔹	Velocity 🔻
Custom Vectors	Velocity Magnitude 🗸 🗸
Vectors of	Surfaces Filter Text
Custom Vectors	air-inlet
	axis-5
Save Output Parameter	fuel-inlet
	interior-4
	nozzle
	outer-wall
	pressure-outlet-9
	Area-Weighted Average (m/s)
	3.305419
Compute W	/rite Close Help

- 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:

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

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.

11

1. Enable the NOx model.

Setup
$$\rightarrow$$
 Models \rightarrow Species \rightarrow NOx $\stackrel{\bigcirc}{\rightarrow}$ Edit...

ues	Formation Mo	odel Parameters
Formation Reduction Turbulence Interaction Mode	Thermal	Prompt Fuel N2O Path
Pathways Thermal NOx Prompt NOx Fuel NOx Number of Fuel Streams Fuel Streams Fuel Species [1/5] Ch4 o2 co2 h2o User-Defined Functions NOx Rate none	[O] Model [OH] Model	partial-equilibrium

- 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.

dels			Formation Mo	del Paramet	ters	
Formation Reduct	ion Turbulence Inte	raction Mode	Thermal	Prompt	Fuel	N20 Pat
PDF Mod	etemperature	•	[O] Model	partial-equi	librium	
PDF Typ	ebeta	•	[OH] Model	none		•
	PDF Points 20	•				
Temperature Varianc	etransported	•				
Tmax Optio	global-tmax	•				

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.

	Formation Model Parameters
ormation Reduction Turbulence Interaction Mode	Thermal Prompt Fuel N2O Path
PDF Mode temperature PDF Type beta PDF Points 20 Temperature Variance transported Tmax Option global-tmax	Fuel Carbon Number 1 Equivalence Ratio 0.76

- 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.



Equations
Equations [2/9]
Flow
Turbulence
ch4
o2
co2
h2o
Pollutant no
Temperature Variance
Energy
L
OK Default Cancel Help

- 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 \rightarrow Controls \rightarrow Controls

Solution Controls	
Pseudo Transient Explicit Relaxation Factors	_
0.75	^
h2o	
0.75	
Pollutant no	
1	
Temperature Variance	
1	
Energy	=
0.75	
	-
Default	
Equations Limits Advanced	
Set All Species URFs Together	

- 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.

|--|

Options Print to Console	Equations Residual	Monitor C	heck Converg	ence Absolute Criteria	
V Plot	pollut_no	V		1e-06	
Window	tvar			0.001	
Iterations to Plot	Residual Values	1		Convergence Criterio	n
iterations to Store	Normalize		terations 5	absolute	•
1000 🔄	Scale Compute Lo	cal Scale		Convergence Condi	tions

- 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).

100001 HHH H	File \rightarrow	Write →	Case 8	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 \rightarrow Graphics \rightarrow Contours \rightarrow 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 \rightarrow Reports \rightarrow Surface Integrals...

Surface Integrals	
Report Type	Field Variable
Mass-Weighted Average	N0x 🔻
Custom Vectors	Mass fraction of Pollutant no
Vectors of	Surfaces Filter Text
Custom Vectors	air-inlet
	axis-5
Save Output Parameter	fuel-inlet
	interior-4
	nozzle
	outer-wall
	pressure-outlet-9
	zone-sunace-/
	Mass-Weighted Average
	0.0042108
Compute	rite Close Help

- 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.

E Setup \rightarrow Models \rightarrow Species \rightarrow NOx $\stackrel{\text{D}}{\rightarrow}$ 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)).



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.



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.



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)).







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:

$$NOppm = \frac{NOmole fraction \times 10^{6}}{1 - H_{2}Omole fraction}$$

(13.4)

Note

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

$\blacksquare User Defined \rightarrow Field Functions \rightarrow Custom...$

+	-	X	1	y^x	ABS	Select Operand Field Functions from
INV	sin	COS	tan) n	log10	Species
0	1	2	3	4	SQRT	Mole fraction of h2o
5	б	7	8	9	CE/C	
()	PI	e		DEL	Select

- 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 \rightarrow Graphics \rightarrow Contours \rightarrow 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:

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

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).