Tutorial 13. 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 eddydissipation model in FLUENT.

This tutorial will demonstrate 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 assumes that you are familiar with the menu structure in FLUENT and that you have completed Tutorial 1 . Some steps in the setup and solution procedure will not be shown explicitly.

You may find it helpful to read Chapter 14 of the User's Guide to learn more about chemical reaction modeling. 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 13.1. 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 13.1: 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

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

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.

Setup and Solution

Preparation

- 1. Download species_transport.zip from the Fluent Inc. User Services Center or copy it from the FLUENT documentation CD 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. Start the 2D (2d) version of FLUENT.

Step 1: Grid

1. Read the grid file gascomb.msh.

 $\mathsf{File} \longrightarrow \mathsf{Read} \longrightarrow \mathsf{Case...}$

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

2. Check the grid.

Grid → Check

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

3. Scale the grid.

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

Grid	—→Scale
------	---------

Scale Grid	X	
Scale Factors	Unit Conversion	
× 0.001	Grid Was Created In mm 👻	
Y 0.001	Change Length Units	
Domain Extents		
Xmin (m) 👔 Xmax (m) 1.8		
Ymin (m) 🔋	Ymax (m) 0.225	
Scale Unscale Close Help		

- (a) Select mm from the Grid Was Created In drop-down list in the Unit Conversion group box.
- (b) Click Scale.
- (c) Make sure that Xmax and Ymax are 1.8 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.

- (d) Close the Scale Grid panel.
- 4. Display the grid with the default settings.

 $\mathsf{Display} \longrightarrow \mathsf{Grid}...$

Extra: You can use the right mouse button to probe for grid information in the graphics window. If you click the right mouse button on any node in the grid, information will be displayed in the 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.



Figure 13.2: The Quadrilateral Grid for the Combustor Model

Step 2: Models

1. Define the domain as axisymmetric.

$\boxed{\text{Define}} \longrightarrow \boxed{\text{Models}} \longrightarrow \boxed{\text{Solver}}$

Solver	×
Solver • Pressure Based • Density Based	Formulation Implicit C Explicit
Space C 2D Axisymmetric Axisymmetric Swirl C 3D Velocity Formulation Absolute C Relative	Time Steady Unsteady
Gradient Option Green-Gauss Cell Ba Green-Gauss Node E C Least Squares Cell E	Porous Formulation ased Based Based
ОК	Cancel Help

(a) Select Axisymmetric from the Space list.

- (b) Retain the default settings for the remaining pressure-based solver parameters.
- (c) Click OK to close the Solver panel.
- 2. Enable heat transfer by enabling the energy equation.

 $\boxed{\text{Define}} \longrightarrow \boxed{\text{Models}} \longrightarrow \boxed{\text{Energy}} \dots$

Energy		×
Energy I Energ	y Equatior	1
ОК	Cancel	Help

3. Select the standard k- ϵ turbulence model.

 $\boxed{\mathsf{Define}} \longrightarrow \boxed{\mathsf{Models}} \longrightarrow \mathsf{Viscous}...$

Viscous Model	×
Model Model Inviscid Laminar Spalart-Allmaras (1 eqn) k-epsilon (2 eqn) k-omega (2 eqn) Reynolds Stress (5 eqn) k-epsilon Model Standard RNG Realizable Near-Wall Treatment Standard Wall Functions Non-Equilibrium Wall Functions Enhanced Wall Treatment User-Defined Wall Functions Options Viscous Heating	Model Constants Cmu 09 C1-Epsilon 1.44 C2-Epsilon 1.92 TKE Prandtl Number 1 User-Defined Functions Value tviscosity none Prandtl Numbers TKE Prandtl Number none TDR Prandtl Number none Energy Prandtl Number none Energy Prandtl Number none Value tviscosity
OK Cancel Help	

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

The Viscous Model *panel 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 panel.
- 4. Enable chemical species transport and reaction.

 $\underline{\mathsf{Define}} \longrightarrow \underline{\mathsf{Models}} \longrightarrow \underline{\mathsf{Species}} \longrightarrow \underline{\mathsf{Transport}} \& \operatorname{Reaction} \dots$

Species Model	×	
Model	Mixture Properties	
 Off Species Transport Non-Premixed Combustion Premixed Combustion Partially Premixed Combustion 	Mixture Material methane-air View Number of Volumetric Species 5	
© Composition PDF Transport	Turbulence-Chemistry Interaction	
Reactions Volumetric Wall Surface Particle Surface	 Laminar Finite-Rate Finite-Rate/Eddy-Dissipation Eddy-Dissipation EDC 	
Options Inlet Diffusion Diffusion Energy Source Full Multicomponent Diffusion Thermal Diffusion		
OK Apply Cancel Help		

(a) Select Species Transport from the Model list.

The Species Model panel 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 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 Materials panel (see Step 3: Materials). (d) Select Eddy-Dissipation from the Turbulence-Chemistry Interaction list.

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 panel.

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



Note that 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):



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 4: Boundary Conditions.

Step 3: 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. You will 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.

The Materials panel will display the mixture material (methane-air) that was selected in the Species Model panel. The properties for this mixture material have been copied from the FLUENT database and will be modified in the following steps.

Materials			×
Name	Material Type		Order Materials By
methane-air	mixture	-	• Name
Chemical Formula	Fluent Mixture Materials		C Chemical Formula
	methane-air	•	Fluent Database
	Mixture		User-Defined Database
	none	-	
Properties		-1-1	
Mixture Species	names 🔻 Edit	1	
Reaction	eddy-dissipation <u>Edit</u>		
Mechanism	hanism reaction-mechs 💌 Edit		
Density (kg/m3)	incompressible-ideal-gas 💽 Edit	•	
Change/Create Delete Close Help			

Define \longrightarrow Materials...

(a) Retain the default selection of mixture in the Material Type drop-down list.

(b) Click the Edit... button to the right of the Mixture Species drop-down list to open the Species panel.

Species	\mathbf{X}
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
ОК	ncel Help

You can add or remove species from the mixture material as necessary using the Species panel.

i. Retain the default selections in the Selected Species selection list.

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

ii. Click Cancel to close the Species panel.

(c) Click the Edit... button to the right of the Reaction drop-down list to open the Reactions panel.

Reactions	X	
Mixture methane-air	Total Number of Reactions 1	
Reaction Name ID Reaction Type reaction-1 1 • · Volumetric	C Wall Surface C Particle Surface	
Number of Reactants 2	Number of Products 2	
Stoich. Rate Species Coefficient Exponent	Species Stoich. Rate Coefficient Exponent	
ch4 • 1 1	co2 - 1 0	
02 2 1	▼ h2o ▼ 2 Ø	
Arrhenius Rate	Mixing Rate	
Pre-Exponential Factor 2.119e+	11 A 4 B 0.5	
Activation Energy (j/kgmol) 2.027e+	08	
Temperature Exponent	—	
Third-Body Efficiencies Specify		
Pressure-Dependent Reaction Speci	ify	
ОКС	Cancel Help	

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 panel. 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.) See the User's Guide for details.

- i. Retain the default values in the Mixing Rate group box.
- ii. Click OK to close the $\mathsf{Reactions}$ constants.
- (d) Retain the selection of incompressible-ideal-gas from the Density drop-down list.

Materials		
Name	Material Type	Order Materials By
methane-air	mixture	Name
Chemical Formula	Fluent Mixture Materials	Chemical Formula
	methane-air	Fluent Database
	Mixture	User-Defined Database
	none	·
Properties		
Cp (j/kg-k)	constant 🗾 Edit	
	1000	
Thermal Conductivity (w/m-k)	constant 👻 Edit	
	0.0454	
Viscosity (kg/m-s)	constant 💌 Edit	
	1.72e-05	
Mass Diffusivity (m2/s)	constant-dilute-appx 🗾 Edit	
	2.88e-05	
]	_	
Change/Create Delete Close Help		

(e) Select constant from the Cp drop-down list and enter $1000~\mathrm{J/kg}-\mathrm{K}$ for the specific heat value.

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

- (f) Click Change/Create to accept the material property settings.
- (g) Close the Materials panel.

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 6: Solution with Varying Heat Capacity.

Step 4: Boundary Conditions

Define →Boundary Conditions...

Boundary Conditions 🛛 🔀		
Zone	Туре	
fluid-1	axis 🔼	
pressure-outlet-9	inlet-vent	
symmetry-5	intake-fan	
velocity-inlet-6	interface mass-flow-inlet	
wall-2	outflow	
wall-7	outlet-vent pressure-far-field	
	pressure-inlet	
	pressure-outlet	
5		
]		
Set Copy Close Help		

1. Convert the symmetry zone to the axis type.

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

- (a) Select symmetry-5 from the Zone list.
- (b) Select axis from the Type list.

Scroll up the list to find axis.

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 panel will open and display the default name for the newly created axis zone. Click OK to continue.

Axis	×
Zone Name	
axis-5	

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

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

Velocity Inlet
Zone Name
air-inlet
Momentum Thermal Radiation Species DPM Multiphase UDS
Velocity Specification Method Magnitude, Normal to Boundary
Reference Frame Absolute
Velocity Magnitude (m/s) 0.5 constant
Turbulence
Specification Method Intensity and Hydraulic Diameter
Turbulent Intensity (%) 10
Hydraulic Diameter (m) 0.44
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 dropdown list in the Turbulence group box.
- (d) Retain the default value of 10% for $\mathsf{Turbulent}\ \mathsf{Intensity}.$
- (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 $0.23~{\rm for}~o2$ in the Species Mass Fractions group box.

Veloci	y Inlet					
Zone	Name					
air-	inlet					
Мот	entum Thermal Ra	diation Species DPM	Multiphase UDS			
Spec	ies Mass Fractions					
ch4	0	constant 👻 🚽				
02	0.23	constant 👻				
co2	0	constant 🗸				
h2o	0	constant 🗸	-			
ĺ.		_	-			
OK Cancel Help						

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

Velocity Inlet	×
Zone Name	
fuel-inlet	
Momentum Thermal Radiation Species DPM Multiphase U	JDS
Velocity Specification Method Magnitude, Normal to Boundary	•
Reference Frame Absolute	•
Velocity Magnitude (m/s) 80 constant	•
Turbulence	
Specification Method Intensity and Hydraulic Diameter	•
Turbulent Intensity (%) 10	
Hydraulic Diameter (m) 0.01	
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 dropdown 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.

Velocity Inlet					
Zone Name					
fuel-inlet					
Momentum Thermal Ra	diation Species DPM Multiphase UDS				
Species Mass Fractions					
ch4 1	constant 🗸 📥				
o2 g	constant 👻				
co2 g	constant 🚽				
h20 0	constant 🚽				
	OK Cancel Help				

(h) Click OK to close the Velocity Inlet panel.

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

Pressure Outlet
Zone Name pressure-outlet-9
Momentum Thermal Radiation Species DPM Multiphase UDS
Gauge Pressure (pascal) 👔 🔹 🔹
Backflow Direction Specification Method Normal to Boundary
Target Mass Flow Rate
Turbulence
Specification Method Intensity and Hydraulic Diameter
Backflow Turbulent Intensity (%) 10
Backflow Hydraulic Diameter (m) 0.45
OK Cancel Help

- (a) Retain the default value of $0\ {\rm Pa}$ for ${\sf Gauge\ Pressure}.$
- (b) Select Intensity and Hydraulic Diameter from the Specification Method dropdown list in the Turbulence group box.
- (c) Retain the default value of 10% for 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 $0.23~{\rm for}~o2$ in the Species Mass Fractions group box.

Pressu	ire Outlet		×				
Zone	Name						
pres	sure-outlet-9						
Мот	nentum Thermal Ra	adiation Species DPM Multiphase UDS					
Spec	cies Mass Fractions						
ch4	0	constant 🗸					
02	0.23	constant 🗸					
co2	0	constant 🗸					
h2o	0	constant 🗸					
ĺ.		_					
		OK Cancel Help					

(g) Click OK to close the $\mathsf{Pressure}$ Outlet panel.

The Backflow values in the Pressure Outlet panel are utilized only when backflow occurs at the pressure outlet. Reasonable values should always be assigned, since backflow may occur during intermediate iterations and could affect the solution stability.

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

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

Wall										
Zone Name outer-wall Adjacent Cell Zo	one									
fluid-1 Momentum T	hermal	Radiation	Species	DPM	Multi	phase	UDS	1		
Thermal Condi Heat Flux Temperatu Convection Radiation Mixed Material Name aluminum	itions ure n	Heat	Te Generatio	empera	iture (k) (w/m3)	300	Wall Thi	ckness	constant 6 (m) 0 constant	•
			OK	C	ancel	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 from the Thermal Conditions list.
 - ii. Retain the default value of $300\ \mathrm{K}$ for Temperature.
- (c) Click OK to close the Wall panel.

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

Wall		
Zone Name		
nozzle		
Adjacent Cell Zone		
fluid-1		
Momentum There	mal Radiation Species DPM	Multiphase UDS
Thermal Condition	IS	
Heat Flux	Heat Flux	× (w/m2) 0 constant 👻
C Temperature		Wall Thickness (m) g
C Radiation	Heat Generation Rate	e (w/m3) g
C Mixed		
Material Name		
aluminum	Edit	
	OK	ancel Help

(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 from the Thermal Conditions list.
 - ii. Retain the default value of $0~\mathrm{W/m^2}$ for $\mathsf{Heat}\ \mathsf{Flux},$ so that the wall is adiabatic.
- (c) Click OK to close the Wall panel.
- 7. Close the Boundary Conditions panel.

Step 5: Initial Solution with Constant Heat Capacity

- 1. Initialize the field variables.
 - Solve \longrightarrow Initialize \longrightarrow Initialize...

Solution Initialization
Compute From Reference Frame
all-zones Relative to Cell Zone Absolute
Initial Values
Gauge Pressure (pascal) 👔 📥
Axial Velocity (m/s) 👔 🔤
Radial Velocity (m/s) 👔
Turbulent Kinetic Energy (m2/s2) 0.05120805
Init Reset Apply Close Help

- (a) Select all-zones from the Compute From drop-down list.
- (b) Click **Init** to initialize the variables.
- (c) Close the Solution Initialization panel.

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

The default under-relaxation parameters in 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.

Solve	\longrightarrow	Controls	\longrightarrow Solution
00110	-		ooracioniii

Solution Controls		\mathbf{X}			
Equations 📃 🗐	Under-Relaxation Factors				
Flow Turbulence	ch4	0.95			
ch4	02	9.05			
o2 co2		0.75			
h2o Epergy	C02	0.95			
Litergy	h2o	0.95			
Pressure-Velocity Coupling Discretization					
SIMPLE	Pressure	Standard 🗸			
	Momentum	First Order Upwind 👻			
	Turbulent Kinetic Energy	First Order Upwind 🔹			
	Turbulent Dissipation Rate	First Order Upwind			
OK Default Cancel Help					

(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.

(b) Click OK to close the Solution Controls panel.

3. Enable the plotting of residuals during the calculation.

 $\fbox{Solve} \longrightarrow \fbox{Monitors} \longrightarrow \r{Residual} \dots$

Residual Monit	ors				X
Options	Storage			Plotting	
✓ Print✓ Plot	lter	ations 10	00 🔺	Wind	low 0
	Normalizati	on		Iterations	1000 🛨
	□ N	ormalize	Scale	Axes	Curves
	Convergenc	e Criterio	n		
	absolute		•		
Residual	Ch Monitor Co	eck nvergenc	Absolute e Criteria	-	
continuity			0.001	_	
x-velocity	~		0.001		
y-velocity	V	V	0.001		
energy		$\overline{\mathbf{v}}$	1e-06		
k		•	0.001		
OK Plot Renorm Cancel Help					

- (a) Enable Plot in the Options group box.
- (b) Click OK to close the Residual Monitors panel.
- 4. Save the case file (gascomb1.cas.gz).

 $\mathsf{File} \longrightarrow \mathsf{Write} \longrightarrow \mathsf{Case...}$

- (a) Enter gascomb1.cas.gz for Case File.
- (b) Make sure the Write Binary Files option is enabled to produce a smaller, unformatted binary file.
- (c) Click OK close the Select File dialog box.

5. Start the calculation by requesting 500 iterations.

Solve \longrightarrow Iterate...

Iterate 🛛 🗙		
Iteration		
Number of Iterations 500		
Reporting Interval 1		
UDF Profile Update Interval 1		
Iterate Apply Close Help		

The solution will converge in approximately 300 iterations.

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

 $\mathsf{File} \longrightarrow \mathsf{Write} \longrightarrow \mathsf{Case} \And \mathsf{Data...}$

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

7. Review the current state of the solution by displaying filled contours of temperature (Figure 13.3).

Display \longrightarrow Contours...

Contours		
Options	Contours of	
Filled	Temperature 👻	
☑ Node Values ☑ Global Range		
Auto Range	Min (k)	Max (k)
Clip to Range	300	3078.064
Draw Profiles	Surfaces	= =
	air-inlet	~
Levels Setup	axis-5	=
	interior-4	
Surface Name Pattern	nozzle	~
	Surface Types	II.
1	axis	^
Match	clip-surf	
	fan	~
Display Compute Close Help		

- (a) Enable Filled in the Options group box.
- (b) Select Temperature... and Static Temperature from the Contours of drop-down lists.
- (c) Click Display and close the Contours panel.



Figure 13.3: 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 6: 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 FLUENT database to recompute the solution.

1. Enable composition dependence of the specific heat.



Materials		
Name	Material Type	Order Materials By
methane-air	mixture	• Name
Chemical Formula	Fluent Mixture Materials	Chemical Formula
]	methane-air 🗸	Fluent Database
	Mixture	User-Defined Database
	none	,
Properties		
Cp (j/kg-k) п	ixing-law 🗸 Edit	
Ϊ		
Thermal Conductivity (w/m-k) c	unstant	
0	. 0454	
Viscosity (kg/m-s) c	instant	
1	.72e-05	
Mass Diffusivity (m2/s) c	instant-dilute-appx 👻 Edit	
2	.88e-05	
, ,	▲	
Change/Create Delete Close Help		

- (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.

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

Define \longrightarrow Materials...

Materials		X
Name	Material Type	Order Materials By
carbon-dioxide	fluid 🗸	• Name
Chemical Formula	Fluent Fluid Materials	C Chemical Formula
co2	carbon-dioxide (co2)	Fluent Database
	Mixture	User-Defined Database
	methane-air 🗨	
Properties		
Cp (j/kg-k)	piecewise-polynomial 🔹 Edit	<u> </u>
Molecular Weight (kg/kgmol)	constant 🗨 Edit	
	44.00995	
Standard State Enthalpy (j/kgmol)	gmol) constant 💌 Edit	
	-3.935324e+08	
Standard State Entropy (j/kgmol-k) constant		
	213720.2	•
Change/Create	Delete Close Hel	p

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

By selecting the fluid material type, you will have access to all of the species in the mixture.

(b) Select carbon-dioxide (co2) from the Fluent Fluid Materials drop-down list.

(c) Select piecewise-polynomial from the Cp drop-down list in the Properties group box.

The Piecewise-Polynomial Profile panel will open.

Piecewise-Polynomial Profile		
DefineIn Terms ofRangesCpTemperature2		
RangeMinimumMaximumCoefficients1130010005		
Coefficients 1 429.9289 2 1.874473 3 -0.001966485 4 1.297251e-06		
5 -3.999956e-10 6 7 8		
OK Cancel Help		

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

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

- ii. Click OK to close the Piecewise-Polynomial Profile panel.
- (d) Click Change/Create in the Materials panel to accept the change in properties.
- 3. In a similar manner, enable temperature dependence of specific heat for the remaining species (CH₄, N₂, O₂, and H₂O). Close the Materials panel when you are finished.

 $\mathsf{Define} \longrightarrow \mathsf{Materials...}$

Remember to click **Change/Create** to accept the change for each species.

4. Request 500 more iterations.

Solve \longrightarrow Iterate...

The residuals will jump significantly as the solution adjusts to the new specific heat representation. The solution will converge after approximately 230 additional iterations.

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

$$\mathsf{File} \longrightarrow \mathsf{Write} \longrightarrow \mathsf{Case} \And \mathsf{Data...}$$

Step 7: Postprocessing

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

1. Display filled contours of temperature (Figure 13.4).

Display \longrightarrow Contours...

- (a) Make sure that Filled is enabled in the Options group box.
- (b) Make sure that Temperature... and Static Temperature are selected in the Contours of drop-down lists.
- (c) Click Display.



Figure 13.4: 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.

2. Display filled contours of specific heat (Figure 13.5).

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

Display \longrightarrow Contours...

- (a) Select Properties... and Specific Heat (Cp) from the Contours of drop-down lists.
- (b) Click Display and close the Contours panel.



Figure 13.5: Contours of Specific Heat

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. 3. Display velocity vectors (Figure 13.6).



Vectors	X	
Options	Vectors of	
Global Range	Color by	
Clip to Range	Velocity	
Draw Grid	Velocity Magnitude Image: Magnitude Min Max	
Style arrow 💌	0	
Scale 0.01	Surfaces =	
Skip 🔋 🔶	air-inlet axis-5	
Vector Options	fuel-inlet 🔤	
Custom Vectors	nozzle outer-wall	
Surface Name Pattern	Surface Types 📃 📃	
	axis	
Match	exhaust-fan fan 🗸	
Display Compute Close Help		

- (a) Enter 0.01 for Scale.
- (b) Click the Vector Options... button to open the Vector Options panel.

Vector Options		
 □ In Plane ✓ Fixed Length ✓ X Component ✓ Y Component ✓ Z Component 	Scale Head Ø.1 Color	
Apply Close Help		

i. Enable the Fixed Length option.

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 panel.

(c) Click Display and close the Vectors panel.



Figure 13.6: Velocity Vectors: Variable C_p

4. Display filled contours of stream function (Figure 13.7).

Display \longrightarrow Contours...

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

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

5. Display filled contours of mass fraction for CH_4 (Figure 13.8).

Display \longrightarrow Contours...

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



Figure 13.7: Contours of Stream Function: Variable C_p



Figure 13.8: Contours of CH_4 Mass Fraction

6. In a similar manner, display the contours of mass fraction for the remaining species O_2 , CO_2 , and H_2O (Figures 13.9, 13.10, and 13.11). Close the **Contours** panel when all of the species have been displayed.



Figure 13.9: Contours of O_2 Mass Fraction



Figure 13.10: Contours of CO_2 Mass Fraction



Figure 13.11: Contours of H₂O Mass Fraction

7. Determine the average exit temperature.

Report \longrightarrow Surface Integrals...

Surface Integrals	X		
Surface Integrals Report Type Mass-Weighted Averaç - Surface Types = = axis clip-surf exhaust-fan fan Surface Name Pattern Match	Field Variable Temperature Static Temperature Surfaces air-inlet axis-5 fuel-inlet interior-4 nozzle outer-wall		
pressure-outlet-9 Mass-Weighted Average (k) 1795.74 Compute Write 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 1796 K.

8. Determine the average exit velocity.

Report \longrightarrow Surface Integrals...

Surface Integrals	×	
Report Type Area-Weighted Average Surface Types = = axis clip-surf	Field Variable Velocity Velocity Magnitude Surfaces	
Surface Name Pattern	air-iniet axis-5 fuel-inlet interior-4 nozzle outer-wall pressure-outlet-9	
	Area-Weighted Average (m/s) 3.137691	
Compute Write 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

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

(c) Click Compute.

The Area-Weighted Average field will show that the exit velocity is approximately 3.14 m/s.

(d) Close the Surface Integrals panel.

Step 8: NO_x Prediction

In this section you will extend the 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.

Define — Models	\longrightarrow Species	—→NOx…
-----------------	---------------------------	--------

NOx Model		
Models	Formation Model Parameters	
Formation Reduction Turbulence Interaction	Thermal Prompt Fuel N20 Path	
Pathways ✓ Thermal NO ✓ Prompt NO 「 Fuel NO 「 N2O Intermediate	[O] Model equilibrium [OH] Model none	
User-Defined Functions		
NOx Rate none		
Apply Close Help		

(a) Enable the Thermal NO option in the Pathways group box.

An Information dialog box will open, warning about the SNCR model. Click OK in the Information dialog box to continue.

Information 🛛 🛛 🗙					
(į)	Warning! Empty Reagent Species List SNCR Model Disabled				
	ΟΚ				

- (b) Enable the **Prompt NO** option.
- (c) Click the Turbulence Interaction tab.

NOx Model						
Models Formation Model Parameters						
Formation Reduction Turbulence Interaction	Thermal Prompt Fuel N2O Path					
Turbulence Interaction Mode PDF Mode temperature Beta PDF Points 10	[O] Model partial-equilibrium [OH] Model none					
Apply Close Help						

i. Select temperature from the PDF Mode drop-down list in the Turbulence Interaction Mode group box.

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 timeaveraged reaction rates.

ii. Retain the default value of 10 for Beta PDF Points.

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

(d) Select partial-equilibrium from the [O] Model drop-down list 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.

NOx Model						
Models Formation Model Parameters						
Formation Reduction Turbulence Interaction	Thermal Prompt Fuel N20 Path					
Turbulence Interaction Mode PDF Mode temperature Beta PDF Points 10	Fuel Species = = ch4 o2 co2 h2o Fuel Carbon Number 1 Equivalence Ratio 8.76					
Apply Close Help						

- i. Select ch4 from the Fuel Species selection list.
- ii. Retain the default value of 1 for Fuel Carbon Number.
- iii. 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.

An Information dialog box will open. Click OK to continue.

- (g) Close the NOx Model panel.
- 2. Enable the calculation of only the NO species, and set the under-relaxation factor for this equation.

Solve —	Controls	\longrightarrow Solution
---------	----------	----------------------------

Solution Controls		X			
Equations 📃 🗐	Under-Relaxation Factors				
Flow	co2	0.95			
ch4	h2a				
02		0.95			
102 h20	Pollutant no	1			
Pollutant no	Energy	1			
Energy		-			
Pressure-Velocity Coupling	Discretization				
SIMPLE	Pressure	Standard 🗸			
	Momentum	First Order Upwind			
Turbulent Kinetic Energy First Order Upwind					
Turbulent Dissipation Rate First Order Upwind					
OK Default Cancel Help					

- (a) Deselect all variables except Pollutant no from the Equations selection list.
- (b) Enter 1 for Pollutant no in the Under-Relaxation Factors group box. Scroll down the Under-Relaxation Factors group box to find Pollutant no.
- (c) Click OK to close the Solution Controls panel.

You will predict NO_x formation in a "postprocessing" mode, with the flow field, temperature, and hydrocarbon combustion species concentrations fixed. Thus, 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. Reduce the convergence criterion for the NO species equation.

Solve \longrightarrow Monitors \longrightarrow Residual...

Residual Moni	itors	X
Options	Storage	Plotting
✓ Print✓ Plot	Iterations 1000	Window 🛛 🛨
	Normalization	Iterations 1000
	🗆 Normalize 🗹 Scale	Axes Curves
	Convergence Criterion	
	absolute 🗸	
Residual	Check Absolute Monitor Convergence Criteria	
pollut_no	V V 1e-06	
		~
0	K Plot Renorm C	ancel Help

- (a) Enter 1e-06 for the Absolute Criteria of pollut_no.
- (b) Click OK to close the Residual Monitors panel.
- 4. Request 50 more iterations.

Solve \longrightarrow Iterate...

The solution will converge in approximately 10 iterations.

5. Save the new case and data files (gascomb3.cas and gascomb3.dat).

6. Review the solution by displaying contours of NO mass fraction (Figure 13.12).

Display \longrightarrow Contours...

- (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 panel.



Figure 13.12: Contours of NO Mass Fraction: Prompt and Thermal NO_x Formation

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

7. Calculate the average exit NO mass fraction.

Report \rightarrow Surface Integrals	Report	→Surface	Integrals
--	--------	----------	-----------

Surface Integrals	×				
Report Type Mass-Weighted Averaç	Field Variable				
Surface Types	Mass fraction of Pollutant no Surfaces air-inlet axis-5 fuel-inlet interior-4 nozzle outer-wall pressure-outlet-9				
Mass-Weighted Average 0.004635032					
Compute	te 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 dropdown lists.
- (c) Make sure 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 0.00464.

- (e) Close the Surface Integrals panel.
- 8. Disable the prompt NO_x mechanism in preparation for solving for thermal NO_x only.

 $\boxed{\text{Define}} \longrightarrow \boxed{\text{Models}} \longrightarrow \boxed{\text{Species}} \longrightarrow \boxed{\text{NOx...}}$

- (a) Click the Formation tab and disable the Prompt NO option.
- (b) Click Apply and close the NOx Model panel.

An Information dialog box will open. Click OK to continue.

9. Request 50 iterations.

Solve \longrightarrow Iterate...

The solution will converge in less than 10 iterations.

10. Review the thermal NO_x solution by viewing contours of NO mass fraction (Figure 13.13).

Display \longrightarrow Contours...

- (a) Make sure that NOx... and Mass fraction of Pollutant no are selected from the Contours of drop-down list.
- (b) Click Display and close the Contours panel.



Figure 13.13: Contours of NO Mass Fraction: Thermal NO_x Formation

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

11. Compute the average exit NO mass fraction with only thermal NO_x formation. Report \longrightarrow Surface Integrals...

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 0.00460.

12. Solve for prompt NO_x production only.

 $\boxed{\mathsf{Define}} \longrightarrow \boxed{\mathsf{Models}} \longrightarrow \boxed{\mathsf{Species}} \longrightarrow NOx...$

- (a) Disable the Thermal NO option in the Pathways group box.
- (b) Enable the **Prompt NO** option.

(c) Click Apply and close the NOx Model panel.

An Information dialog box will open. Click OK to continue.

13. Request 50 iterations.

Solve \longrightarrow Iterate...

The solution will converge in less than 10 iterations.

14. Review the prompt NO_x solution by viewing contours of NO mass fraction (Figure 13.14).

Display \longrightarrow Contours...



Figure 13.14: 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.

15. Compute the average exit NO mass fraction with only prompt NO_x formation.

Report \longrightarrow Surface Integrals...

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 7.131e-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.

16. Use a custom field function to compute NO parts per million (ppm). NO ppm will be computed from the following equation:

$$NO ppm = \frac{NO mole fraction \times 10^6}{1 - H_2O mole fraction}$$
(13.4)

Custom	Field Fu	nction C	alculato	r			X
Definitio	on 					4 1- 5 - 60- 3	
moret-	-polluc	-pollu	canc-0	* 10	0 / (1 - MO10+-N2O)	
+	-	×	1	y^x	ABS	Select Operand Field Functions from	
INV	sin	cos	tan	In	log10	Field Functions	
0	1	2	3	4	SQRT	Species 💌	
5	6	7	8	9	CE/C	Mole fraction of h2o	
(]	PI	е	•	DEL	Select	
New Function Name no-ppm							
Define Manage Close Help							

Define \longrightarrow Custom Field Functions...

- (a) Select NOx... and Mole fraction of Pollutant no from the Field Functions dropdown 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 panel.

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, see Tutorial 1 for an example.

- (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 panel.

17. Display contours of NO ppm (Figure 13.15).

Display \longrightarrow Contours...

- (a) Select Custom Field Functions... and no-ppm in the Contours of drop-down lists. Scroll up the list to find Custom Field Functions....
- (b) Click Display and close the Contours panel.



Figure 13.15: Contours of NO ppm: Prompt NO_x Formation

The contours closely resemble the mass fraction contours (Figure 13.14), as expected.

Summary

In this tutorial you used 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 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.

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

	Peak Temp.	Exit Temp.	Exit Velocity
	(K)	(K)	(m/s)
Constant C_p	3078	2198	3.84
Variable C_p	2302	1796	3.14

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 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.

See Chapter 15 of the User's Guide for more details on the nonpremixed combustion model.

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

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

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

See Section 13.3 of the User's Guide and Tutorial 5 for details on radiation modeling.

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 grid. Grid adaption can also ensure that the solution is independent of the grid. These steps are demonstrated in Tutorial 1.