

Syngas Combustion in a Round-Jet Burner

Introduction

This model simulates turbulent combustion of syngas (synthesis gas) in a simple round jet burner. Syngas is a gas mixture, primarily composed of hydrogen, carbon monoxide and carbon dioxide. The name syngas relates to its use in creating synthetic natural gas.

The model set up corresponds to the one studied by Couci et al. in Ref. 1. The temperature and composition resulting from the nonpremixed combustion in the burner setup have also been experimentally investigated by Barlow and coworkers (Ref. 2 and Ref. 3) as a part of the International Workshop on Measurement and Computation of Turbulent Nonpremixed Flames (Ref. 4). The model is solved in COMSOL Multiphysics by combining a Reacting Flow and a Heat Transfer in Fluids interface.

Model Definition

The burner studied in this model consists of a straight pipe placed in a slight co-flow. The gas phase fuel is fed through the pipe using an inlet velocity of 76 m/s, while the co-flow velocity outside of pipe is 0.7 m/s. At the pipe exit, the fuel gas mixes with the co-flow, creating an unconfined circular jet. The gas fed through the tube consists of three compounds typical of syngas; carbon monoxide (CO), hydrogen (H_2) and nitrogen (N_2) . The co-flow gas consists of air. At the pipe exit, the fuel is ignited. Since the fuel and oxidizer enter the reaction zone separately, the resulting combustion is of the nonpremixed type. A continuous reaction requires that the reactants and the oxidizer are mixed to stoichiometric conditions. In this set-up the turbulent flow of the jet effectively mixes the fuel from the pipe with the co-flowing oxygen. Furthermore the mixture needs to be continuously ignited. In this burner the small recirculation zones generated by the pipe wall thickness provide the means to decelerate hot product gas. The recirculation zones hereby promote continuous ignition of the oncoming mixture and stabilizes the flame at the pipe orifice. In experiments (Ref. 4) no lift-off or localized extinction of the flame has been observed.

In the current model, the syngas combustion is modeled using two irreversible reactions:

$$CO + 0.5O_2 \rightarrow CO_2$$

 $H_2 + 0.5O_2 \rightarrow H_2O$ (1)

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This assumption of a complete oxidation of the fuel corresponds to one of the approaches used in Ref. 1. The mass transport in the reacting jet is modeled by solving for the mass fractions of six species; the five species participating in the reactions and nitrogen N_2 originating in the co-flowing air.

The Reynolds number for the jet, based on the inlet velocity and the inner diameter of the pipe, is approximately 16700, indicating that the jet is fully turbulent. Under these circumstances, both the mixing and the reactions processes in the jet are significantly influenced by the turbulent nature of the flow. To account for the turbulence when solving for the flow field, the k- ω turbulence model is applied.

Taking advantage of the symmetry, a two-dimensional model using a cylindrical coordinate system is solved.

TURBULENT REACTION RATE

When using a turbulence model in a Reacting Flow interface, the production rate (SI unit: $kg/(m^3 \cdot s)$) of species *i* resulting from reaction *j* is modeled as the minimum of the mean-value-closure reaction rate and the eddy-dissipation-model rate:

$$R_{ij} = v_{ij}M_i \cdot \min[r_{\text{MVC},j}, r_{\text{ED},j}]$$

The mean-value-closure rate is the kinetic reaction rate expressed using the mean mass fractions. This corresponds to the characteristic reaction rate for reactions which are slow compared to the turbulent mixing, or the reaction rate in regions with negligible turbulence levels. This can be quantified through the Damköhler number, which compares the turbulent time scale (τ_T) to the chemical time scale (τ_c). The mean-value-closure is appropriate for low Damköhler numbers:

$$Da = \frac{\tau_T}{\tau_c} \ll 1$$

The reaction rate defined by the eddy-dissipation model (Ref. 5) is:

$$r_{\text{ED},j} = \frac{\alpha_j}{\tau_{\text{T}}} \rho \cdot \min\left[\min\left(\frac{\omega_r}{v_{rj}M_r}\right), \beta \sum_p \left(\frac{\omega_p}{v_{pj}M_p}\right)\right]$$
(2)

where τ_T (SI unit: s) is the mixing time scale of the turbulence, ρ is the mixture density (SI unit: kg/m³), ω is the species mass fraction, ν denotes the stoichiometric coefficients, and M is the molar mass (SI unit: kg/mol). Properties of reactants of the reaction are indicated using a subscript r, while product properties are denoted by a subscript p.

The eddy-dissipation model assumes that both the Reynolds and Damköhler numbers are sufficiently high for the reaction rate to be limited by the turbulent mixing time scale τ_{T} . A global reaction can then at most progress at the rate at which fresh reactants are mixed, at the molecular level, by the turbulence present. The reaction rate is also assumed to be

limited by the deficient reactant; the reactant with the lowest local concentration. The model parameter β specifies that product species is required for reaction, modeling the activation energy. For gaseous non-premixed combustion the model parameters have been found to be (Ref. 5):

$$\alpha = 4, \beta = 0.5$$

In the current model the molecular reaction rate of the reactions is assumed to be infinitely fast. This is achieved in the model by prescribing unrealistically high rate constants for the reactions. This implies that the production rate is given solely by the turbulent mixing in Equation 2.

It should be noted that the eddy-dissipation model is a robust but simple model for turbulent reactions. The reaction rate is governed by a single time scale, the turbulent mixing time-scale. For this reason, the reactions studied should be limited to global one step (as in Equation 1), or two step reactions.

HEAT OF REACTION

The heat of reaction, or change in enthalpy, following each reaction is defined from the heat of formation of the products and reactants:

$$\Delta H_{\rm r} = \sum_{\rm products} \Delta H_{\rm f} - \sum_{\rm reactants} \Delta H_{\rm f}$$

The heat of formations for each species is given in Table 1 (based on Ref. 6). Since the heat of formation of the products is lower than that of the reactants, both reactions are exothermic and release heat. The heat release is included in the model by adding a Heat Source feature to the Heat Transfer in Fluids interface. The heat source (SI unit: W/m^3) applied is defined as:

$$q = r_{\rm ED,1} \Delta H_{\rm r1} + r_{\rm ED,2} \Delta H_{\rm r2}$$

SPECIES	$\Delta H_{ m f}$ (cal/mol)	$C_{ m p}$ (cal/(mol·K)	$C_{ m p}$ (cal/(mol·K)	$C_{ m p}$ (cal/(mol·K)
	T = 298 K	T = 300 K	T = 1000 K	T = 2000 K
N_2	0	6.949	7.830	8.601
H_2	0	6.902	7.209	8.183
O_2	0	7.010	8.350	9.032
H_2O	-57.80	7.999	9.875	12.224

TABLE I: SPECIES ENTHALPY OF FORMATION AND HEAT CAPACITY

4 | SYNGAS COMBUSTION IN A ROUND-JET BURNER

SPECIES	$\Delta H_{ m f}$ (cal/mol) T = 298 K	C _p (cal/(mol·K) Т = 300 К	C _p (cal/(mol·K) T = 1000 К	$C_{\rm p} \; ({\rm cal/(mol \cdot K)})$ T = 2000 K
со	-26.420	47.259	6.950	7.948
CO_2	-94.061	51.140	8.910	12.993

TABLE I: SPECIES ENTHALPY OF FORMATION AND HEAT CAPACITY

HEAT CAPACITY

The temperature in the jet increases significantly due to the heat release following the reactions, this is one of the defining features of combustion. For an accurate prediction of the temperature it is important to account for the temperature dependence of the species heat capacities. In the model, interpolation functions for the heat capacity at constant pressure, $C_{p,i}$ (SI unit: cal/(mol·K)), for each species are defined using the values at three different temperatures given in Table 1. The heat capacity of the mixture, $c_{p,mix}$ (SI unit: J/(kg·K)), is computed as a mass fraction weighted mean of the individual heat capacities:

$$c_{\rm p, mix} = \sum_{i} \frac{\omega_i C_{\rm p,i}}{M_i}$$

SOLUTION PROCEDURE

The syngas combustion model is solved in three steps.

- I Use an initial submodel to solve for isothermal turbulent flow in a straight pipe with the same diameter as the burner. The fully developed flow at the pipe outlet is then used as inlet condition for the burner.
- **2** Solve for the turbulent and reacting, but isothermal, flow in the round jet burner configuration.
- **3** Include the heat transfer and solve for the fully coupled reacting flow, using the previous solution as initial condition.

Using several solution steps is vital for a robust solution procedure when solving models with a high degree of coupling. This is the case for turbulent reacting flow including heat transfer.

Results and Discussion

The resulting velocity field in the non-isothermal reacting jet is visualized in Figure 1. The expansion and development of the hot free jet is clearly seen. The turbulent mixing in the outer parts of the jet acts to accelerate fluid originating in the co-flow, and incorporate it

in the jet. This is commonly referred to as entrainment and can be observed in the co-flow streamlines which bend towards the jet downstream of the orifice.



Figure 1: The velocity magnitude and flow paths (streamlines) of the reacting jet.

The temperature in the jet is shown in Figure 2 where a revolved data set has been used to emphasize the structure of the round jet. The maximum temperature in the jet is seen to be approximately 1960 K. The carbon dioxide mass fraction in the reacting jet is plotted in Figure 3. The formation of CO_2 takes place in the outer shear layer of the jet. This is where the fuel from the pipe encounters oxygen in the co-flow and reacts. The reactions are promoted by the turbulent mixing in the jet shear layer. It is also seen that the CO_2 formation starts just outside of the pipe. This is also the case for the temperature increase in Figure 2. This implies that there is no lift-off and the flame is attached to the pipe.

In Figure 4, Figure 5, and Figure 6 the results reached in the model are compared with the experimental results of Barlow and coworkers (Ref. 2, Ref. 3, and Ref. 4). In Figure 4 the jet temperature is further examined and compared with the experiments. In the left panel the temperature along the centerline is plotted. It is seen that the maximum temperature predicted in the model is close to that in the experiment. However in the model the temperature profile is shifted in the downstream direction. This is most likely due to the fact that radiation has not been included in the model.

In the right panel of Figure 4 temperature profiles at 20 and 50 pipe diameters downstream of the pipe exit are compared with the experiments. The axial velocity of the jet is compared with the experimental results in Figure 5, using the same down stream positions. The axial velocity is found to compare well with the experimental values at both positions.

In Figure 6 the species concentration along the jet centerline is analyzed and compared with the experimental results. For some species, N_2 , and CO_2 , the axial mass fraction development agrees well with the experimental results. For the fuel species CO and H_2 a fair agreement is observed. For the remaining species, O_2 and H_2O , the trend appears correct but the profiles are shifted downstream, as was the case with the temperature. The reason for the discrepancy in the mass fractions can in part be attributed to the fact that radiation is not included, but the accuracy is probably also significantly influenced by the simplified reaction scheme and the eddy-dissipation model.



Figure 2: Jet temperature shown using a revolved data set.



Figure 3: CO_2 mass fraction in the reacting jet.



Figure 4: Jet temperature along the centerline (left), and radially at two different positions downstream of the pipe exit (right) scaled by the inlet temperature. The centerline and radial distance is scaled by the inner diameter of the pipe. Model results are plotted using lines, while experimental results are indicated using symbols. The downstream positions are defined in terms of the inner diameter of the pipe (d).



Figure 5: Axial velocity at two different positions downstream of the pipe exit, scaled by the inlet velocity. The radial distance is scaled by the inner diameter of the pipe. Model results are plotted using lines, while experimental results are indicated using symbols.



Figure 6: Species mass fractions along the jet centerline. The centerline distance is scaled by the

inner diameter of the pipe. Model results are plotted using lines, while experimental results are indicated using symbols.

References

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3. M. Flury, Experimentelle Analyse der Mischungstruktur in turbulenten nicht vorgemischten Flammen, Ph.D. Thesis, ETH Zurich, 1998.

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5. B.F. Magnussen and B.H. Hjertager, "On Mathematical Modeling of Turbulent Combustion with Special Emphasis on Soot Formation and Combustion," *16th Symp.* (*Int.*) on Combustion. Comb. Inst., Pittsburg, Pennsylvania, pp.719–729, 1976.

6. A. Frassoldati, T. Faravelli, and E. Ranzi, "The Ignition, Combustion and Flame Structure of Carbon Monoxide/Hydrogen Mixtures. Note 1: Detailed Kinetic Modeling of Syngas Combustion Also in Presence of Nitrogen Compounds," *Int. J. Hydrogen Energy*, vol. 32, pp. 3471–3485, 2007.

Application Library path: Chemical_Reaction_Engineering_Module/ Reactors_with_Mass_and_Heat_Transfer/round_jet_burner

Modeling Instructions

From the File menu, choose New.

NEW

In the New window, click Model Wizard.

MODEL WIZARD

- I In the Model Wizard window, click 2D Axisymmetric.
- 2 In the Select Physics tree, select Fluid Flow>Single-Phase Flow>Turbulent Flow> Turbulent Flow, k-ω (spf).
- 3 Click Add.
- 4 Click Study.
- 5 In the Select Study tree, select Preset Studies>Stationary.
- 6 Click Done.

GLOBAL DEFINITIONS

Parameters

- I On the Home toolbar, click Parameters.
- 2 In the Settings window for Parameters, locate the Parameters section.
- **3** Click Load from File.
- **4** Browse to the model's Application Libraries folder and double-click the file round_jet_burner_params.txt.

GEOMETRY I

Rectangle 1 (r1)

- I On the Geometry toolbar, click Primitives and choose Rectangle.
- 2 In the Settings window for Rectangle, locate the Size and Shape section.
- **3** In the **Width** text field, type Di/2.
- 4 In the **Height** text field, type Di*200.
- 5 Right-click Rectangle I (rI) and choose Build Selected.
- 6 Click the Zoom Extents button on the Graphics toolbar.

DEFINITIONS

For easier visualization of the slender geometry, disable preserve aspect ratio for the view.

View I

In the Model Builder window, expand the Component I (compl)>Definitions node.

Axis

- I In the Model Builder window, expand the View I node, then click Axis.
- 2 In the Settings window for Axis, locate the Axis section.

- 3 From the View scale list, choose Automatic.
- 4 Click the **Zoom Extents** button on the **Graphics** toolbar.

Apply fluid properties for the pipe simulation. An approximate density can be used.

TURBULENT FLOW, $K-\omega$ (SPF)

Fluid Properties 1

- I In the Model Builder window, under Component I (compl)>Turbulent Flow, k-ω (spf) click Fluid Properties I.
- 2 In the Settings window for Fluid Properties, locate the Fluid Properties section.
- **3** From the ρ list, choose **User defined**. In the associated text field, type 1.
- **4** From the μ list, choose **User defined**. In the associated text field, type mu_mix.

Inlet 1

- I On the Physics toolbar, click Boundaries and choose Inlet.
- **2** Select Boundary 2 only.
- 3 In the Settings window for Inlet, locate the Turbulence Conditions section.
- **4** In the $L_{\rm T}$ text field, type 0.07*Di.
- **5** Locate the **Velocity** section. In the U_0 text field, type Ujet.

Outlet I

- I On the Physics toolbar, click Boundaries and choose Outlet.
- **2** Select Boundary **3** only.
- 3 In the Settings window for Outlet, locate the Pressure Conditions section.
- 4 Select the Normal flow check box.

MESH I

Distribution I

- I In the Model Builder window, under Component I (comp1) right-click Mesh I and choose Mapped.
- 2 Right-click Mapped I and choose Distribution.
- **3** Select Boundaries 2 and 3 only.
- 4 In the Settings window for Distribution, locate the Distribution section.
- 5 From the Distribution properties list, choose Predefined distribution type.
- 6 In the Number of elements text field, type 25.

7 In the **Element ratio** text field, type 5.

8 Click Build Selected.

Distribution 2

- I Right-click Mapped I and choose Distribution.
- 2 Select Boundaries 1 and 4 only.
- 3 In the Settings window for Distribution, locate the Distribution section.
- **4** From the **Distribution properties** list, choose **Predefined distribution type**.
- 5 In the Number of elements text field, type 200.
- 6 In the Element ratio text field, type 20.
- 7 Click Build Selected.

Now add a second model for the round reacting jet simulation.

8 On the Home toolbar, click Component and choose Add Component>2D Axisymmetric.

GEOMETRY 2

In the Model Builder window, under Component 2 (comp2) click Geometry 2.

ADD PHYSICS

- I On the Home toolbar, click Add Physics to open the Add Physics window.
- 2 Go to the Add Physics window.
- 3 In the tree, select Chemical Species Transport>Reacting Flow>Turbulent Flow> Turbulent Flow, k-ω.
- 4 Find the Physics interfaces in study subsection. In the table, clear the Solve check box for Study 1.
- 5 Click to expand the Dependent variables section. Locate the Dependent Variables section.In the Number of species text field, type 6.
- 6 In the Mass fractions table, enter the following settings:

wCO
w02
wC02
wH2
wH20
wN2

7 Click Add to Component in the window toolbar.

- 8 Go to the Add Physics window.
- 9 In the tree, select Heat Transfer>Heat Transfer in Fluids (ht).
- 10 Find the Physics interfaces in study subsection. In the table, clear the Solve check box for Study 1.
- II Click Add to Component in the window toolbar.
- 12 On the Home toolbar, click Add Physics to close the Add Physics window.

COMPONENT 2 (COMP2)

On the Home toolbar, click Windows and choose Add Multiphysics.

ADD MULTIPHYSICS

- I Go to the Add Multiphysics window.
- 2 In the tree, select No Coupling Features Available for the Selected Physics Interfaces.
- **3** Find the **Select the physics interfaces you want to couple** subsection. In the table, enter the following settings:

Physics	Couple
Transport of Concentrated Species (tcs)	

- 4 In the tree, select Fluid Flow>Nonisothermal Flow>Turbulent Flow>Turbulent Flow, k-@.
- **5** Find the **Multiphysics couplings in study** subsection. In the table, enter the following settings:

Studies	Solve
Study I	

- 6 Click Add to Component in the window toolbar.
- 7 On the Home toolbar, click Add Multiphysics.

MULTIPHYSICS

- I In the Model Builder window, under Component 2 (comp2)>Multiphysics click Nonisothermal Flow I (nitf1).
- 2 In the Settings window for Nonisothermal Flow, locate the Material Properties section.
- **3** From the **Specify density** list, choose **Custom**.
- **4** From the ρ list, choose **Density (tcs/cdm1)**.
- **5** Locate the **Flow Heating** section. Select the **Include work done by pressure changes** check box.

ADD STUDY

- I On the Home toolbar, click Add Study to open the Add Study window.
- 2 Go to the Add Study window.
- 3 Find the Studies subsection. In the Select Study tree, select Preset Studies>Stationary.
- 4 Click Add Study in the window toolbar.
- 5 On the Home toolbar, click Add Study to close the Add Study window.

DEFINITIONS

Variables 1

- I On the Home toolbar, click Variables and choose Local Variables.
- 2 In the Settings window for Variables, locate the Variables section.
- 3 Click Load from File.
- **4** Browse to the model's Application Libraries folder and double-click the file round_jet_burner_vars.txt.

GEOMETRY 2

Rectangle 1 (r1)

- I On the Geometry toolbar, click Primitives and choose Rectangle.
- 2 In the Settings window for Rectangle, locate the Size and Shape section.
- 3 In the Width text field, type GeomW.
- 4 In the **Height** text field, type GeomH.
- 5 Right-click Rectangle I (rI) and choose Build Selected.

Rectangle 2 (r2)

- I On the Geometry toolbar, click Primitives and choose Rectangle.
- 2 In the Settings window for Rectangle, locate the Size and Shape section.
- **3** In the **Width** text field, type Pth.
- **4** In the **Height** text field, type P1.
- 5 Locate the **Position** section. In the **r** text field, type Di/2.
- 6 Right-click Rectangle 2 (r2) and choose Build Selected.

Chamfer 1 (cha1)

- I On the Geometry toolbar, click Chamfer.
- 2 On the object r2, select Points 3 and 4 only.

- 3 In the Settings window for Chamfer, locate the Distance section.
- 4 In the **Distance from vertex** text field, type Pth*0.15.
- 5 Right-click Chamfer I (chal) and choose Build Selected.
- 6 Click the **Zoom Extents** button on the **Graphics** toolbar.

Bézier Polygon I (b1)

- I On the Geometry toolbar, click Primitives and choose Bézier Polygon.
- 2 Click the **Zoom Extents** button on the **Graphics** toolbar.
- 3 In the Settings window for Bézier Polygon, locate the Polygon Segments section.
- 4 Find the Added segments subsection. Click Add Linear.
- 5 Find the Control points subsection. In row I, set r to GeomW.
- 6 In row 2, set r to GeomW*1.5 and z to GeomH.
- 7 Find the Added segments subsection. Click Add Linear.
- 8 Find the Control points subsection. In row 2, set r to GeomW.
- 9 Right-click Bézier Polygon I (bI) and choose Build Selected.

Union I (uni I)

- I On the Geometry toolbar, click Booleans and Partitions and choose Union.
- 2 Select the objects **b1** and **r1** only.
- 3 In the Settings window for Union, locate the Union section.
- 4 Clear the Keep interior boundaries check box.
- 5 Right-click Union I (unil) and choose Build Selected.

Difference I (dif1)

- I On the Geometry toolbar, click Booleans and Partitions and choose Difference.
- 2 Select the object unil only.
- 3 In the Settings window for Difference, locate the Difference section.
- **4** Find the **Objects to subtract** subsection. Select the **Active** toggle button.
- 5 Select the object **chal** only.
- 6 Right-click Difference I (difl) and choose Build Selected.

Bézier Polygon 2 (b2)

- I On the Geometry toolbar, click Primitives and choose Bézier Polygon.
- 2 In the Settings window for Bézier Polygon, locate the Polygon Segments section.
- 3 Find the Added segments subsection. Click Add Linear.

- 4 Find the Control points subsection. In row I, set r to Di/2 and z to Pl+0.3e-3.
- 5 In row 2, set r to Di and z to GeomH.
- 6 Right-click Bézier Polygon 2 (b2) and choose Build Selected.

Bézier Polygon 3 (b3)

- I On the Geometry toolbar, click Primitives and choose Bézier Polygon.
- 2 In the Settings window for Bézier Polygon, locate the Polygon Segments section.
- 3 Find the Added segments subsection. Click Add Linear.
- 4 Find the **Control points** subsection. In row I, set r to Di/2+Pth and z to Pl+0.3e-3.
- 5 In row 2, set r to 0.04 and z to GeomH.
- 6 Right-click Bézier Polygon 3 (b3) and choose Build Selected.

Form Union (fin)

In the Model Builder window, under Component 2 (comp2)>Geometry 2 right-click Form Union (fin) and choose Build Selected.

Mesh Control Edges 1 (mcel)

- I On the Geometry toolbar, click Virtual Operations and choose Mesh Control Edges.
- 2 On the object fin, select Boundaries 6 and 11 only.
- 3 Right-click Mesh Control Edges I (mcel) and choose Build Selected.
- 4 Click the **Zoom Extents** button on the **Graphics** toolbar.

Form Composite Edges 1 (cme1)

- I On the Geometry toolbar, click Virtual Operations and choose Form Composite Edges.
- 2 On the object mcel, select Boundaries 3 and 11 only.
- 3 Right-click Form Composite Edges I (cmel) and choose Build Selected.

That concludes the geometry for the reacting jet. Now define a coupling variable that can be used to apply the outlet conditions from the previous model to the inlet of the current.

DEFINITIONS

In the Model Builder window, under Component I (compl) click Definitions.

Linear Extrusion 1 (linext1)

- I On the Definitions toolbar, click Component Couplings and choose Linear Extrusion.
- 2 Click in the Graphics window and then press Ctrl+A to select all domains.
- 3 In the Settings window for Linear Extrusion, locate the Source Vertices section.
- **4** Select the **Active** toggle button.

- **5** Select Point 2 only.
- 6 Select the Active toggle button.
- **7** Select Point 4 only.
- 8 Click to expand the **Destination** section. From the **Destination geometry** list, choose **Geometry 2**.
- 9 Locate the **Destination Vertices** section. Select the **Active** toggle button.
- **IO** Select Point 1 only.
- II Select the Active toggle button.
- 12 Select Point 3 only.

TURBULENT FLOW, K-002 (SPF2)

Fluid Properties 1

- I In the Model Builder window, under Component 2 (comp2)>Turbulent Flow, k- ω 2 (spf2) click Fluid Properties I.
- 2 In the Settings window for Fluid Properties, locate the Fluid Properties section.
- **3** From the μ list, choose **User defined**. In the associated text field, type mu_mix.

Inlet 1

- I On the Physics toolbar, click Boundaries and choose Inlet.
- **2** Select Boundary 2 only.
- 3 In the Settings window for Inlet, locate the Velocity section.
- 4 In the U_0 text field, type comp1.linext1(w).
- 5 Locate the Turbulence Conditions section. Click the Specify turbulence variables button.
- **6** In the k_0 text field, type comp1.linext1(k).
- 7 In the ω_0 text field, type comp1.linext1(om).

Inlet 2

- I On the Physics toolbar, click Boundaries and choose Inlet.
- 2 Select Boundaries 9 and 10 only.
- 3 In the Settings window for Inlet, locate the Velocity section.
- 4 Click the **Velocity field** button.

5 Specify the **u**₀ vector as

- **6** Locate the **Turbulence Conditions** section. In the $I_{\rm T}$ text field, type 0.01.
- 7 In the $L_{\rm T}$ text field, type 0.1*Di.

Outlet I

- I On the Physics toolbar, click Boundaries and choose Outlet.
- **2** Select Boundary **3** only.
- 3 In the Settings window for Outlet, locate the Pressure Conditions section.
- 4 Select the Normal flow check box.

TRANSPORT OF CONCENTRATED SPECIES (TCS)

- I In the Model Builder window, under Component 2 (comp2) click Transport of Concentrated Species (tcs).
- 2 In the Settings window for Transport of Concentrated Species, locate the Transport Mechanisms section.
- 3 From the Diffusion model list, choose Fick's law.
- 4 Locate the Species section. From the From mass constraint list, choose wN2.

Transport Properties 1

Apply the temperature from the heat transfer interface.

- I In the Model Builder window, under Component 2 (comp2)> Transport of Concentrated Species (tcs) click Transport Properties I.
- 2 In the Settings window for Transport Properties, locate the Model Input section.
- **3** From the *T* list, choose **Temperature (ht)**.
- **4** Locate the **Density** section. In the $M_{\rm wCO}$ text field, type M_CO.
- **5** In the $M_{\rm wO2}$ text field, type M_02.
- **6** In the $M_{\rm wCO2}$ text field, type M_CO2.
- 7 In the $M_{\rm wH2}$ text field, type M_H2.
- 8 In the $M_{\rm wH2O}$ text field, type M_H2O.
- **9** In the $M_{\rm wN2}$ text field, type M_N2.

Initial Values 1

- I In the Model Builder window, under Component 2 (comp2)> Transport of Concentrated Species (tcs) click Initial Values I.
- 2 In the Settings window for Initial Values, locate the Initial Values section.
- **3** In the $\omega_{0,wCO}$ text field, type 0.
- **4** In the $\omega_{0,wO2}$ text field, type wcf_02.
- **5** In the $\omega_{0,wCO2}$ text field, type **0**.
- **6** In the $\omega_{0,wH2}$ text field, type 0.
- **7** In the $\omega_{0,wH2O}$ text field, type **0**.

Inflow I

- I On the Physics toolbar, click Boundaries and choose Inflow.
- **2** Select Boundary 2 only.
- 3 In the Settings window for Inflow, locate the Inflow section.
- 4 From the Mixture specification list, choose Mole fractions.
- **5** In the $x_{0,wCO}$ text field, type x0_C0.
- **6** In the $x_{0,wO2}$ text field, type x0_02.
- 7 In the $x_{0,wCO2}$ text field, type x0_CO2.
- **8** In the $x_{0,wH2}$ text field, type x0_H2.
- **9** In the $x_{0,wH2O}$ text field, type x0_H2O.

Inflow 2

- I On the Physics toolbar, click Boundaries and choose Inflow.
- **2** Select Boundaries 9 and 10 only.
- 3 In the Settings window for Inflow, locate the Inflow section.
- **4** In the $\omega_{0,wCO}$ text field, type 1e-5.
- **5** In the $\omega_{0,wO2}$ text field, type wcf_02.
- **6** In the $\omega_{0,wCO2}$ text field, type 1e-5.
- **7** In the $\omega_{0,wH2}$ text field, type 1e-5.
- **8** In the $\omega_{0,wH2O}$ text field, type 1e-5.

Outflow I

- I On the Physics toolbar, click Boundaries and choose Outflow.
- **2** Select Boundary **3** only.

Reaction 1

- I On the Physics toolbar, click Domains and choose Reaction.
- 2 Click in the Graphics window and then press Ctrl+A to select all domains.
- 3 In the Settings window for Reaction, locate the Reaction Rate section.
- **4** In the v_{wCO} text field, type -1.
- **5** In the v_{wO2} text field, type -0.5.
- **6** In the v_{wCO2} text field, type 1.

Apply an unrealistically high reaction rate to model the reactions as infinitely fast. In this case the reaction rate will be given by the turbulent mixing.

- 7 Locate the Rate Constants section. In the k^{f} text field, type 1e100.
- 8 Locate the Turbulent Flow section. From the Turbulent-reaction model list, choose Eddydissipation.

Regularization makes the reaction system much easier to converge.

9 Click to expand the Regularization section. Select the Rate expressions check box.

Reaction 2

- I Right-click Reaction I and choose Duplicate.
- 2 In the Settings window for Reaction, locate the Reaction Rate section.
- **3** In the v_{wCO} text field, type 0.
- **4** In the v_{wCO2} text field, type 0.
- **5** In the v_{wH2} text field, type -1.
- **6** In the v_{wH2O} text field, type **1**.

Use the tabulated heat capacities to create interpolation functions, one for each species.

DEFINITIONS

Interpolation 1 (int1)

- I On the Home toolbar, click Functions and choose Local>Interpolation.
- 2 In the Settings window for Interpolation, locate the Definition section.
- **3** In the **Function name** text field, type Cp_CO.
- **4** In the table, enter the following settings:

t	f(t)
300	47.259

t	f(t)
1000	6.950
2000	7.948

- **5** Locate the **Interpolation and Extrapolation** section. From the **Interpolation** list, choose **Piecewise cubic**.
- 6 Locate the Units section. In the Arguments text field, type K.
- 7 In the Function text field, type cal/mol/K.

Plot the resulting interpolation function.

8 Click Plot.

Interpolation 2 (int2)

- I Right-click Interpolation I (intl) and choose Duplicate.
- 2 In the Settings window for Interpolation, locate the Definition section.
- **3** In the **Function name** text field, type Cp_C02.
- **4** In the table, enter the following settings:

t	f(t)
300	51.140
1000	8.910
2000	12.993

Interpolation 3 (int3)

- I Right-click Component 2 (comp2)>Definitions>Interpolation 2 (int2) and choose Duplicate.
- 2 In the Settings window for Interpolation, locate the Definition section.
- **3** In the **Function name** text field, type Cp_H2.
- **4** In the table, enter the following settings:

t	f(t)
300	6.902
1000	7.209
2000	8.183

Interpolation 4 (int4)

I Right-click Component 2 (comp2)>Definitions>Interpolation 3 (int3) and choose Duplicate.

- 2 In the Settings window for Interpolation, locate the Definition section.
- **3** In the **Function name** text field, type Cp_H20.
- **4** In the table, enter the following settings:

t	f(t)
300	7.999
1000	9.875
2000	12.224

Interpolation 5 (int5)

- I Right-click Component 2 (comp2)>Definitions>Interpolation 4 (int4) and choose Duplicate.
- 2 In the Settings window for Interpolation, locate the Definition section.
- **3** In the **Function name** text field, type Cp_N2.
- **4** In the table, enter the following settings:

t	f(t)
300	6.949
1000	7.830
2000	8.601

Interpolation 6 (int6)

- I Right-click Component 2 (comp2)>Definitions>Interpolation 5 (int5) and choose Duplicate.
- 2 In the Settings window for Interpolation, locate the Definition section.
- **3** In the **Function name** text field, type Cp_02.
- **4** In the table, enter the following settings:

t	f(t)
300	7.010
1000	8.350
2000	9.032

Define the mixture heat capacity. It is computed as the mass average of the species capacities. Also define the enthalpy change for each of the reactions included.

Variables I

I In the Model Builder window, under Component 2 (comp2)>Definitions click Variables I.

2 In the Settings window for Variables, locate the Variables section.

3 In the table, enter the following settings:

Name	Expression	Unit	Description
Cp_mix	<pre>tcs.wr_wC0*Cp_C0(T)/M_C0+ tcs.wr_wC02*Cp_C02(T)/M_C02+ tcs.wr_wH2*Cp_H2(T)/M_H2+ tcs.wr_wH20*Cp_H20(T)/M_H20+ tcs.wr_wN2*Cp_N2(T)/M_N2+ tcs.wr_w02*Cp_02(T)/M_02</pre>	J/(kg·K)	Heat capacity, mixture
dH_R1	dH_CO2-(dH_CO+0.5*dH_O2)	J/mol	Enthalpy change reaction 1
dH_R2	dH_H20-(dH_H2+0.5*dH_02)	J/mol	Enthalpy change reaction 2

Now setup the heat transfer interface.

HEAT TRANSFER IN FLUIDS (HT)

On the Physics toolbar, click Transport of Concentrated Species (tcs) and choose Heat Transfer in Fluids (ht).

Fluid I

- I In the Model Builder window, under Component 2 (comp2)>Heat Transfer in Fluids (ht) click Fluid I.
- 2 In the Settings window for Fluid, locate the Heat Conduction, Fluid section.
- 3 From the k list, choose User defined. In the associated text field, type k_mix+Cp_mix* spf2.muT/0.72.
- 4 Locate the Thermodynamics, Fluid section. From the Fluid type list, choose Ideal gas.
- 5 From the Gas constant type list, choose Mean molar mass.
- **6** From the C_p list, choose **User defined**. In the associated text field, type Cp_mix.

Initial Values 1

- I In the Model Builder window, under Component 2 (comp2)>Heat Transfer in Fluids (ht) click Initial Values I.
- 2 In the Settings window for Initial Values, type T0 in the T text field.
- 3 In the Model Builder window, click Heat Transfer in Fluids (ht).

Temperature 1

- I On the Physics toolbar, click Boundaries and choose Temperature.
- 2 Select Boundaries 2, 9, and 10 only.

- 3 In the Settings window for Temperature, locate the Temperature section.
- **4** In the T_0 text field, type T0.

Outflow I

- I On the Physics toolbar, click Boundaries and choose Outflow.
- 2 Select Boundary 3 only.

Heat Source 1

- I On the Physics toolbar, click Domains and choose Heat Source.
- 2 Click in the Graphics window and then press Ctrl+A to select all domains.
- 3 In the Settings window for Heat Source, locate the Heat Source section.
- **4** In the Q_0 text field, type (dH_R1*tcs.treac1.r+dH_R2*tcs.treac2.r).

MESH 2

- I Click the **Zoom Extents** button on the **Graphics** toolbar.
- 2 In the Model Builder window, under Component 2 (comp2) right-click Mesh 2 and choose Edit Physics-Induced Sequence.

Size

- I In the Model Builder window, under Component 2 (comp2)>Mesh 2 click Size.
- 2 In the Settings window for Size, locate the Element Size section.
- 3 Click the **Custom** button.
- 4 Locate the **Element Size Parameters** section. In the **Maximum element size** text field, type 0.05.
- 5 In the Maximum element growth rate text field, type 1.12.
- 6 In the Resolution of narrow regions text field, type 5.

Size 1

- I In the Model Builder window, under Component 2 (comp2)>Mesh 2 click Size I.
- 2 In the Settings window for Size, locate the Element Size section.
- 3 Click the **Custom** button.
- **4** Locate the **Element Size Parameters** section. Select the **Resolution of narrow regions** check box.
- **5** In the associated text field, type **5**.
- 6 Click Build Selected.

Size 2

- I In the Model Builder window, right-click Mesh 2 and choose Size.
- 2 In the Settings window for Size, locate the Element Size section.
- 3 Click the **Custom** button.
- **4** Locate the **Geometric Entity Selection** section. From the **Geometric entity level** list, choose **Boundary**.
- **5** Select Boundaries 1, 13, and 14 only.
- 6 Locate the Element Size Parameters section. Select the Maximum element size check box.
- 7 In the associated text field, type 0.01.
- 8 Select the Maximum element growth rate check box.
- 9 In the associated text field, type 1.04.

Free Triangular 1

- I In the Model Builder window, under Component 2 (comp2)>Mesh 2 click Free Triangular I.
- 2 In the Settings window for Free Triangular, click to expand the Scale geometry section.
- 3 Locate the Scale Geometry section. In the z-direction scale text field, type 0.5.

Boundary Layer Properties 1

- I In the Model Builder window, expand the Boundary Layers I node, then click Boundary Layer Properties I.
- 2 In the Settings window for Boundary Layer Properties, locate the Boundary Layer Properties section.
- **3** In the Number of boundary layers text field, type 6.
- 4 Click Build All.

Solve the fully developed turbulent pipe flow set up in Component I.

STUDY I

Solution I (soll)

- I On the Study toolbar, click Show Default Solver.
- 2 In the Settings window for Solution, click Compute.

Use the second study to solve the axially symmetric jet flow in **Component 2** using the fully developed turbulent outlet profiles as inlet conditions for the pipe.

STUDY 2

Step 1: Stationary

- I In the Model Builder window, expand the Solution I (soll) node, then click Study 2> Step I: Stationary.
- 2 In the Settings window for Stationary, locate the Physics and Variables Selection section.
- **3** In the table, clear the **Solve for** check box for **Turbulent Flow**, **k**-ω (**spf**) and **Heat Transfer** in **Fluids** (**ht**).
- 4 Click to expand the Values of dependent variables section. Locate the Values of Dependent Variables section. Find the Values of variables not solved for subsection. From the Settings list, choose User controlled.
- 5 From the Method list, choose Solution.
- 6 From the Study list, choose Study I, Stationary.

Adjust the CFL-number controller parameters to speed up convergence. Also, solve the temperature coupled with the velocity and pressure for increased robustness and convergence rate.

Solution 2 (sol2)

- I On the Study toolbar, click Show Default Solver.
- 2 In the Model Builder window, expand the Solution 2 (sol2) node.
- 3 In the Model Builder window, expand the Study 2>Solver Configurations> Solution 2 (sol2)>Stationary Solver I node.
- 4 In the Model Builder window, under Study 2>Solver Configurations>Solution 2 (sol2)> Stationary Solver I click Segregated I.
- 5 In the Settings window for Segregated, locate the General section.
- 6 In the PID regulator-Proportional text field, type 0.65.
- 7 In the PID regulator-Derivative text field, type 0.025.
- 8 In the Target error estimate text field, type 0.1.
- 9 In the Model Builder window, under Study 2>Solver Configurations>Solution 2 (sol2)> Stationary Solver I>Segregated I click Velocity u2, Pressure p2.
- 10 In the Settings window for Segregated Step, locate the General section.
- II Under Variables, click Add.
- **12** In the **Add** dialog box, In the **Variables** list, choose

Wall temperature (comp2.nitf1.TWall_d), Wall temperature (comp2.nitf1.TWall_u), and Temperature (comp2.T).

I3 Click OK.

- I4 In the Model Builder window, under Study 2>Solver Configurations>Solution 2 (sol2)> Stationary Solver I>Segregated I click Segregated Step 2.
- **IS** In the **Settings** window for **Segregated Step**, click to expand the **Method and termination** section.
- 16 Locate the Method and Termination section. In the Number of iterations text field, type 2.
- **I7** In the **Damping factor** text field, type **0.4**.
- 18 In the Model Builder window, under Study 2>Solver Configurations>Solution 2 (sol2)> Stationary Solver I>Segregated I right-click Segregated Step 3 and choose Disable.

Solution 2 (sol2)

- I In the Model Builder window, collapse the Study 2>Solver Configurations> Solution 2 (sol2) node.
- 2 In the Model Builder window, click Solution 2 (sol2).
- 3 In the Settings window for Solution, click Compute.

Now move on to post process the result from the nonisothermal jet. Start by creating a mirrored 2D data set as well as a revolved 3D data set.

RESULTS

Mirror 2D I

- I On the Results toolbar, click More Data Sets and choose Mirror 2D.
- 2 In the Settings window for Mirror 2D, locate the Data section.
- 3 From the Data set list, choose Study 2/Solution 2 (4) (sol2).

Revolution 2D 1

- I In the Model Builder window, under Results>Data Sets click Revolution 2D I.
- 2 In the Settings window for Revolution 2D, click to expand the Revolution layers section.
- 3 Locate the **Revolution Layers** section. In the **Revolution angle** text field, type 180.

Revolution 2D 3

- I Right-click Results>Data Sets>Revolution 2D I and choose Duplicate.
- 2 In the Settings window for Revolution 2D, locate the Data section.
- 3 From the Data set list, choose Study 2/Solution 2 (4) (sol2).

Create two cut lines at fixed heights from the pipe exit.

Cut Line 2D I

- I On the **Results** toolbar, click **Cut Line 2D**.
- 2 In the Settings window for Cut Line 2D, locate the Data section.
- 3 From the Data set list, choose Mirror 2D I.
- 4 Locate the Line Data section. From the Line entry method list, choose Point and direction.
- 5 Find the **Point** subsection. In the **y** text field, type P1+20*Di.
- 6 Click to expand the Advanced section. Find the Space variable subsection. In the x text field, type r_mirr20.

Cut Line 2D 2

- I Right-click Cut Line 2D I and choose Duplicate.
- 2 In the Settings window for Cut Line 2D, locate the Line Data section.
- **3** Find the **Point** subsection. In the **y** text field, type P1+50*Di.
- 4 Locate the Advanced section. Find the Space variable subsection. In the x text field, type r_mirr50.

Now apply the mirror data set to the existing plot groups.

Velocity (spf2)

- I In the Model Builder window, under Results click Velocity (spf2).
- 2 In the Settings window for 2D Plot Group, locate the Data section.
- 3 From the Data set list, choose Mirror 2D I.
- 4 On the Velocity (spf2) toolbar, click Plot.
- 5 In the Model Builder window, expand the Velocity (spf2) node.

Streamline 1

- I Right-click Results>Velocity (spf2) and choose Streamline.
- 2 In the Settings window for Streamline, locate the Streamline Positioning section.
- **3** From the **Positioning** list, choose **Uniform density**.
- **4** In the **Separating distance** text field, type **0.035**.
- 5 Locate the Coloring and Style section. From the Color list, choose Gray.
- 6 On the Velocity (spf2) toolbar, click Plot.
- 7 Click the **Zoom Extents** button on the **Graphics** toolbar.

Pressure (spf2)

I In the Model Builder window, under Results click Pressure (spf2).

- 2 In the Settings window for 2D Plot Group, locate the Data section.
- 3 From the Data set list, choose Mirror 2D I.
- 4 On the Pressure (spf2) toolbar, click Plot.

Wall Resolution (spf2)

- I In the Model Builder window, under Results click Wall Resolution (spf2).
- 2 In the Settings window for 2D Plot Group, locate the Data section.
- 3 From the Data set list, choose Mirror 2D I.
- 4 On the Wall Resolution (spf2) toolbar, click Plot.

Mass Fraction (tcs)

- I In the Model Builder window, under Results click Mass Fraction (tcs).
- 2 In the Settings window for 2D Plot Group, locate the Data section.
- 3 From the Data set list, choose Mirror 2D I.
- **4** Locate the **Plot Settings** section. From the **Color** list, choose **White**.
- 5 On the Mass Fraction (tcs) toolbar, click Plot.

Surface

- I In the Model Builder window, expand the Mass Fraction (tcs) node, then click Surface.
- 2 In the Settings window for Surface, locate the Expression section.
- **3** In the **Expression** text field, type wC02.
- 4 On the Mass Fraction (tcs) toolbar, click Plot.
- 5 Click the Zoom Extents button on the Graphics toolbar.

Velocity (spf2) 1

- I In the Model Builder window, under Results click Velocity (spf2) I.
- 2 In the Settings window for 3D Plot Group, locate the Plot Settings section.
- 3 Clear the Plot data set edges check box.

Temperature, 3D (ht)

- I In the Model Builder window, under Results click Temperature, 3D (ht).
- 2 In the Settings window for 3D Plot Group, locate the Plot Settings section.
- **3** Clear the **Plot data set edges** check box.
- 4 On the Temperature, 3D (ht) toolbar, click Plot.

Import the experimental data files. The files corresponds to the ones published online (Ref. 2) by R. Barlow and co-workers. The name of the model, round_jet_burner, has been prepended to the file names.

Table I

- I On the **Results** toolbar, click **Table**.
- 2 In the Settings window for Table, locate the Data section.
- 3 Click Import.
- 4 Browse to the model's Application Libraries folder and double-click the file round_jet_burner_chnAclY.fav.

TABLE

- I Go to the Table window.
- 2 Right-click Table I and choose Rename.
- 3 In the Rename Table dialog box, type Centerline data in the New label text field.
- 4 Click OK.

RESULTS

Table 2

- I On the **Results** toolbar, click **Table**.
- 2 In the Settings window for Table, locate the Data section.
- 3 Click Import.
- 4 Browse to the model's Application Libraries folder and double-click the file round_jet_burner_chnAd20Y.fav.

TABLE

- I Go to the Table window.
- 2 Right-click Table 2 and choose Rename.
- **3** In the **Rename Table** dialog box, type z/Di = 20, radial data in the **New label** text field.
- 4 Click OK.

RESULTS

Table 3

I On the **Results** toolbar, click **Table**.

- 2 In the Settings window for Table, locate the Data section.
- 3 Click Import.
- 4 Browse to the model's Application Libraries folder and double-click the file round_jet_burner_chnAd50Y.fav.

TABLE

- I Go to the Table window.
- 2 Right-click Table 3 and choose Rename.
- **3** In the **Rename Table** dialog box, type z/Di = 50, radial data in the **New label** text field.
- 4 Click OK.

RESULTS

Table 4

- I On the **Results** toolbar, click **Table**.
- 2 In the Settings window for Table, locate the Data section.
- 3 Click Import.
- 4 Browse to the model's Application Libraries folder and double-click the file round_jet_burner_seq1420.dat.

TABLE

- I Go to the Table window.
- 2 Right-click Table 4 and choose Rename.
- 3 In the **Rename Table** dialog box, type z/Di = 20, radial velocity data in the **New label** text field.
- 4 Click OK.

RESULTS

Table 5

- I On the **Results** toolbar, click **Table**.
- 2 In the Settings window for Table, locate the Data section.
- 3 Click Import.
- 4 Browse to the model's Application Libraries folder and double-click the file round_jet_burner_seq1450.dat.

TABLE

- I Go to the Table window.
- 2 Right-click Table 5 and choose Rename.
- 3 In the **Rename Table** dialog box, type z/Di = 50, radial velocity data in the **New label** text field.
- 4 Click OK.

RESULTS

- ID Plot Group 13
- I On the Results toolbar, click ID Plot Group.
- 2 In the Settings window for ID Plot Group, locate the Data section.
- 3 From the Data set list, choose Study 2/Solution 2 (4) (sol2).

Line Graph 1

- I Right-click ID Plot Group 13 and choose Line Graph.
- 2 Select Boundary 1 only.
- 3 In the Settings window for Line Graph, locate the y-Axis Data section.
- **4** In the **Expression** text field, type T/T0.
- 5 Locate the x-Axis Data section. From the Parameter list, choose Expression.
- 6 In the Expression text field, type (z-P1)/Di.
- 7 Click to expand the Coloring and style section. Locate the Coloring and Style section.From the Color list, choose Black.
- 8 Click to expand the Legends section. Select the Show legends check box.
- 9 From the Legends list, choose Manual.

IO In the table, enter the following settings:

Legends

Model

Table Graph 1

- I In the Model Builder window, under Results right-click ID Plot Group 13 and choose Table Graph.
- 2 In the Settings window for Table Graph, locate the Data section.
- 3 From the x-axis data list, choose r(mm).
- 4 From the Plot columns list, choose Manual.

- 5 In the Columns list, select T(K).
- 6 Click to expand the **Preprocessing** section. Find the **x-axis column** subsection. From the **Preprocessing** list, choose **Linear**.
- 7 In the Scaling text field, type 1/(Di*1000).
- 8 Find the y-axis columns subsection. From the Preprocessing list, choose Linear.
- 9 In the Scaling text field, type 1/T0.
- **10** Locate the **Coloring and Style** section. Find the **Line style** subsection. From the **Line** list, choose **None**.
- II From the Color list, choose Black.
- 12 Find the Line markers subsection. From the Marker list, choose Square.
- **I3** From the **Positioning** list, choose **In data points**.
- 14 Click to expand the Legends section. Select the Show legends check box.
- **I5** From the **Legends** list, choose **Manual**.
- **I6** In the table, enter the following settings:

Legends

Exp.

ID Plot Group 13

- I Right-click ID Plot Group I3 and choose Rename.
- 2 In the Rename ID Plot Group dialog box, type T @ centerline in the New label text field.
- 3 Click OK.
- 4 In the Settings window for ID Plot Group, locate the Plot Settings section.
- 5 Select the x-axis label check box.
- 6 In the associated text field, type (z-Pl)/Di.
- 7 Select the y-axis label check box.
- 8 In the associated text field, type T/T0.
- 9 Locate the Axis section. Select the Manual axis limits check box.
- **IO** In the **x minimum** text field, type 10.
- II In the **x maximum** text field, type 120.
- **12** In the **y minimum** text field, type 0.5.
- **I3** In the **y maximum** text field, type **8**.

- 14 Click to expand the Title section. From the Title type list, choose Manual.
- IS In the Title text area, type Temperature along the centerline.
- **I6** On the **T @** centerline toolbar, click **Plot**.

ID Plot Group 14

- I On the Home toolbar, click Add Plot Group and choose ID Plot Group.
- 2 In the Settings window for ID Plot Group, locate the Data section.
- 3 From the Data set list, choose None.

Line Graph 1

- I Right-click ID Plot Group 14 and choose Line Graph.
- 2 In the Settings window for Line Graph, locate the Data section.
- 3 From the Data set list, choose Cut Line 2D I.
- 4 Locate the y-Axis Data section. In the Expression text field, type T/T0.
- 5 Locate the x-Axis Data section. From the Parameter list, choose Expression.
- 6 In the Expression text field, type r_mirr20/Di.
- 7 Click to expand the Coloring and style section. Locate the Coloring and Style section.From the Color list, choose Black.
- 8 Click to expand the Legends section. Select the Show legends check box.
- 9 From the Legends list, choose Manual.
- **IO** In the table, enter the following settings:

Legends

z/Di = 20, Model

Line Graph 2

- I Right-click Results>ID Plot Group 14>Line Graph I and choose Duplicate.
- 2 In the Settings window for Line Graph, locate the Data section.
- 3 From the Data set list, choose Cut Line 2D 2.
- 4 Locate the x-Axis Data section. In the Expression text field, type r_mirr50/Di.
- **5** Locate the **Coloring and Style** section. Find the **Line style** subsection. From the **Line** list, choose **Dashed**.
- 6 Locate the Legends section. In the table, enter the following settings:

Legends

z/Di = 50, Model

7 On the ID Plot Group 14 toolbar, click Plot.

Table Graph 1

- I In the Model Builder window, under Results right-click ID Plot Group 14 and choose Table Graph.
- 2 In the Settings window for Table Graph, locate the Data section.
- **3** From the Table list, choose z/Di = 20, radial data.
- 4 From the x-axis data list, choose r(mm).
- 5 From the Plot columns list, choose Manual.
- 6 In the Columns list, select T(K).
- 7 Click to expand the Preprocessing section. Find the x-axis column subsection. From the Preprocessing list, choose Linear.
- 8 In the Scaling text field, type 1/(Di*1000).
- 9 Find the y-axis columns subsection. From the Preprocessing list, choose Linear.
- **IO** In the **Scaling** text field, type 1/TO.
- II Click to expand the **Coloring and style** section. Locate the **Coloring and Style** section. Find the **Line style** subsection. From the **Line** list, choose **None**.
- 12 From the Color list, choose Black.
- 13 Find the Line markers subsection. From the Marker list, choose Square.
- 14 From the Positioning list, choose In data points.
- 15 Locate the Legends section. Select the Show legends check box.
- 16 From the Legends list, choose Manual.
- **I7** In the table, enter the following settings:

Legends

z/Di = 20, Exp

Table Graph 2

- I Right-click Results>ID Plot Group 14>Table Graph I and choose Duplicate.
- 2 In the Settings window for Table Graph, locate the Data section.
- **3** From the **Table** list, choose **z/Di = 50**, **radial data**.
- 4 Locate the **Coloring and Style** section. Find the **Line markers** subsection. From the **Marker** list, choose **Triangle**.

5 Locate the **Legends** section. In the table, enter the following settings:

Legends

z/Di = 50, Exp

ID Plot Group 14

- I In the Model Builder window, under Results right-click ID Plot Group 14 and choose Rename.
- 2 In the Rename ID Plot Group dialog box, type T @ z/Di = 20, 50 in the New label text field.
- 3 Click OK.
- 4 In the Settings window for ID Plot Group, locate the Title section.
- 5 From the Title type list, choose Manual.
- 6 In the Title text area, type Temperature downstream of the pipe exit.
- 7 Locate the Plot Settings section. Select the x-axis label check box.
- **8** In the associated text field, type r/Di.
- 9 Select the y-axis label check box.
- **IO** In the associated text field, type T/TO.
- II Locate the Axis section. Select the Manual axis limits check box.
- **12** In the **x minimum** text field, type 10.
- **I3** In the **x maximum** text field, type 10.
- **I4** In the **y minimum** text field, type **0.5**.
- **I5** In the **y maximum** text field, type **8**.
- **I6** On the **T @ z/Di = 20, 50** toolbar, click **Plot**.

T @ z/Di = 20, 50.1

- I In the Model Builder window, under Results right-click T @ z/Di = 20, 50 and choose Duplicate.
- 2 Right-click T @ z/Di = 20, 50.1 and choose Rename.
- **3** In the **Rename ID Plot Group** dialog box, type uz @ z/Di = 20, 50 in the **New label** text field.

4 Click OK.

Line Graph 1

I In the Model Builder window, expand the Results>uz @ z/Di = 20, 50 node, then click Line Graph I.

- 2 In the Settings window for Line Graph, locate the y-Axis Data section.
- 3 In the Expression text field, type w2/Ujet.

Line Graph 2

- I In the Model Builder window, under Results>uz @ z/Di = 20, 50 click Line Graph 2.
- 2 In the Settings window for Line Graph, locate the y-Axis Data section.
- 3 In the Expression text field, type w2/Ujet.

Table Graph 1

- I In the Model Builder window, under Results>uz @ z/Di = 20, 50 click Table Graph I.
- 2 In the Settings window for Table Graph, locate the Data section.
- 3 From the x-axis data list, choose Fblgr.
- 4 From the Table list, choose z/Di = 20, radial velocity data.
- **5** In the **Columns** list, select **uz**.
- 6 Locate the **Preprocessing** section. Find the **y-axis columns** subsection. From the **Preprocessing** list, choose **Linear**.
- 7 In the Scaling text field, type 1/Ujet.

Table Graph 2

- I In the Model Builder window, under Results>uz @ z/Di = 20, 50 click Table Graph 2.
- 2 In the Settings window for Table Graph, locate the Data section.
- 3 From the x-axis data list, choose Fblgr.
- **4** From the Table list, choose z/Di = 50, radial velocity data.
- 5 In the Columns list, select uz.
- 6 Locate the **Preprocessing** section. Find the **y-axis columns** subsection. From the **Preprocessing** list, choose **Linear**.
- 7 In the Scaling text field, type 1/Ujet.

uz @ z/Di = 20, 50

- I In the Model Builder window, under Results click uz @ z/Di = 20, 50.
- 2 In the Settings window for ID Plot Group, locate the Title section.
- 3 In the Title text area, type Axial velocity downstream of the pipe exit.
- 4 Locate the Plot Settings section. In the y-axis label text field, type uz/Ujet.
- 5 Locate the Axis section. In the x minimum text field, type -10.
- 6 In the **x maximum** text field, type 10.

- 7 In the **y minimum** text field, type -0.25.
- 8 In the **y maximum** text field, type 1.25.
- 9 On the uz @ z/Di = 20, 50 toolbar, click Plot.
- **IO** Locate the **Title** section. From the **Title type** list, choose **None**.
- T @ centerline 1
- I In the Model Builder window, under Results right-click T @ centerline and choose Duplicate.
- 2 Right-click T @ centerline I and choose Rename.
- 3 In the Rename ID Plot Group dialog box, type CO, N2 @ centerline in the New label text field.
- 4 Click OK.
- 5 In the Settings window for ID Plot Group, locate the Title section.
- 6 In the Title text area, type Mass fraction along the centerline.
- 7 Locate the Plot Settings section. In the y-axis label text field, type wCO, wN2.
- 8 Locate the Axis section. In the y minimum text field, type -0.05.
- 9 In the y maximum text field, type 1.
- IO On the CO, N2 @ centerline toolbar, click Plot.
- II Click to expand the Legend section. From the Position list, choose Middle right.

Line Graph 1

- I In the Model Builder window, expand the Results>CO, N2 @ centerline node, then click Line Graph I.
- 2 In the Settings window for Line Graph, locate the y-Axis Data section.
- **3** In the **Expression** text field, type wCO.
- 4 Locate the Legends section. In the table, enter the following settings:

Legends

CO, Model

Table Graph 1

- I In the Model Builder window, under Results>CO, N2 @ centerline click Table Graph I.
- 2 In the Settings window for Table Graph, locate the Data section.
- **3** In the **Columns** list, select **YCO**.

- **4** Locate the **Preprocessing** section. Find the **y-axis columns** subsection. In the **Scaling** text field, type **1**.
- 5 Locate the Legends section. In the table, enter the following settings:

Legends

CO, Exp.

6 On the CO, N2 @ centerline toolbar, click Plot.

Line Graph 2

- I In the Model Builder window, under Results>CO, N2 @ centerline right-click Line Graph I and choose Duplicate.
- 2 In the Settings window for Line Graph, locate the y-Axis Data section.
- **3** In the **Expression** text field, type wN2.
- 4 Click to expand the **Coloring and style** section. Locate the **Coloring and Style** section. Find the **Line style** subsection. From the **Line** list, choose **Dashed**.
- **5** Locate the **Legends** section. In the table, enter the following settings:

Legends

N2, Model

Table Graph 2

- I In the Model Builder window, under Results>CO, N2 @ centerline right-click Table Graph I and choose Duplicate.
- 2 In the Settings window for Table Graph, locate the Data section.
- 3 In the Columns list, select YN2.
- 4 Locate the Coloring and Style section. Find the Line markers subsection. From the Marker list, choose Triangle.
- 5 Locate the Legends section. In the table, enter the following settings:

Legends

N2, Exp

6 On the CO, N2 @ centerline toolbar, click Plot.

CO, N2 @ centerline I

- I In the Model Builder window, under Results right-click CO, N2 @ centerline and choose Duplicate.
- 2 Right-click CO, N2 @ centerline I and choose Rename.

- **3** In the **Rename ID Plot Group** dialog box, type H2, H2O @ centerline in the **New label** text field.
- 4 Click OK.

Line Graph 1

- I In the Model Builder window, expand the Results>H2, H20 @ centerline node, then click Line Graph I.
- 2 In the Settings window for Line Graph, locate the y-Axis Data section.
- **3** In the **Expression** text field, type wH2.
- 4 Locate the Legends section. In the table, enter the following settings:

Legends

H2, Model

Table Graph 1

- I In the Model Builder window, under Results>H2, H20 @ centerline click Table Graph I.
- 2 In the Settings window for Table Graph, locate the Data section.
- 3 In the Columns list, select YH2.
- 4 Locate the Legends section. In the table, enter the following settings:

Legends

H2, Exp.

Line Graph 2

- I In the Model Builder window, under Results>H2, H20 @ centerline click Line Graph 2.
- 2 In the Settings window for Line Graph, locate the y-Axis Data section.
- **3** In the **Expression** text field, type wH20.
- 4 Locate the Legends section. In the table, enter the following settings:

Legends

H2O, Model

Table Graph 2

- I In the Model Builder window, under Results>H2, H20 @ centerline click Table Graph 2.
- 2 In the Settings window for Table Graph, locate the Data section.
- 3 In the Columns list, select YH20.

4 Locate the Legends section. In the table, enter the following settings:

Legends

H2O, Exp

H2, H2O @ centerline

- I In the Model Builder window, under Results click H2, H20 @ centerline.
- 2 In the Settings window for ID Plot Group, locate the Plot Settings section.
- 3 In the y-axis label text field, type wH2, wH20.
- 4 Locate the Axis section. In the y maximum text field, type 0.15.
- **5** In the **y minimum** text field, type -0.02.
- 6 Locate the Legend section. From the Position list, choose Upper right.
- 7 On the H2, H20 @ centerline toolbar, click Plot.

H2, H2O @ centerline I

- I In the Model Builder window, right-click H2, H20 @ centerline and choose Duplicate.
- 2 Right-click H2, H2O @ centerline I and choose Rename.
- **3** In the **Rename ID Plot Group** dialog box, type **02**, **C02** @ centerline in the **New label** text field.
- 4 Click OK.

Line Graph I

- I In the Model Builder window, expand the Results>02, CO2 @ centerline node, then click Line Graph I.
- 2 In the Settings window for Line Graph, locate the y-Axis Data section.
- **3** In the **Expression** text field, type w02.
- 4 Locate the Legends section. In the table, enter the following settings:

Legends

02, Model

Table Graph 1

- I In the Model Builder window, under Results>02, CO2 @ centerline click Table Graph I.
- 2 In the Settings window for Table Graph, locate the Data section.
- 3 In the Columns list, select YO2.

4 Locate the Legends section. In the table, enter the following settings:

Legends

02, Exp.

Line Graph 2

- I In the Model Builder window, under Results>02, CO2 @ centerline click Line Graph 2.
- 2 In the Settings window for Line Graph, locate the y-Axis Data section.
- **3** In the **Expression** text field, type wCO2.
- 4 Locate the Legends section. In the table, enter the following settings:

Legends

CO2, Model

Table Graph 2

- I In the Model Builder window, under Results>02, CO2 @ centerline click Table Graph 2.
- 2 In the Settings window for Table Graph, locate the Data section.
- 3 In the Columns list, select YCO2.
- 4 Locate the Legends section. In the table, enter the following settings:

Legends

CO2, Exp

02, CO2 @ centerline

- I In the Model Builder window, under Results click 02, C02 @ centerline.
- 2 In the Settings window for ID Plot Group, locate the Plot Settings section.
- 3 In the y-axis label text field, type w02, wC02.
- 4 Locate the Axis section. In the y minimum text field, type -0.05.
- **5** In the **y maximum** text field, type **0.4**.
- 6 On the 02, CO2 @ centerline toolbar, click Plot.
- 7 Click Plot.

44 | SYNGAS COMBUSTION IN A ROUND-JET BURNER