Created in COMSOL Multiphysics 5.6

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 setup corresponds to the one studied by Couci and others 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 coflow. The gas phase fuel is fed through the pipe using an inlet velocity of 76 m/s, while the coflow velocity outside of pipe is 0.7 m/s. At the pipe exit, the fuel gas mixes with the coflow, 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 coflow 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 setup, the turbulent flow of the jet effectively mixes the fuel from the pipe with the coflowing 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:

$$\mathrm{CO} + 0.5\mathrm{O_2} \rightarrow \mathrm{CO_2}$$

$$\mathrm{H_2} + 0.5\mathrm{O_2} \rightarrow \mathrm{H_2O} \qquad (1)$$

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 coflowing air.

The Reynolds number for the jet, based on the inlet velocity and the inner diameter of the pipe, is approximately 16,700, 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:

$$R_{ij} = \nu_{ij} M_i \cdot \min\left[r_{\mathrm{MVC},j}, r_{\mathrm{ED},j}\right]$$

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 that 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:

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

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

$$r_{\mathrm{ED},j} = \frac{\alpha_j}{\tau_T}\rho \cdot \min\left[\min\left(\frac{\omega_r}{\nu_{rj} M_r}\right), \beta \sum_p \left(\frac{\omega_p}{\nu_{pj} M_p}\right)\right] \qquad (2)$$

where τ_T (SI unit: s) is the mixing time scale of the turbulence, ρ is the mixture density (SI unit: kg/m^3), 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:

$$\Delta H_r = \sum_{\text{products}} \Delta H_f - \sum_{\text{reactants}} \Delta H_f$$

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:

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

TABLE 1: SPECIES ENTHALPY OF FORMATION AND HEAT CAPACITY.

SPECIES	ΔH_f (cal/mol) T = 298 K	C_p (cal/(mol·K) T = 300 K	C_p (cal/(mol·K) T = 1000 K	C_p (cal/(mol·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 1: SPECIES ENTHALPY OF FORMATION AND HEAT CAPACITY.

SPECIES	ΔH_f (cal/mol) T = 298 K	C_p (cal/(mol·K) T = 300 K	C_p (cal/(mol·K) T = 1000 K	C_p (cal/(mol·K) T = 2000 K
CO	-26.420	47.259	6.950	7.948
CO_2	-94.061	51.140	8.910	12.993

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:

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

Results and Discussion

The resulting velocity field in the nonisothermal 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 toward the jet downstream of the orifice.

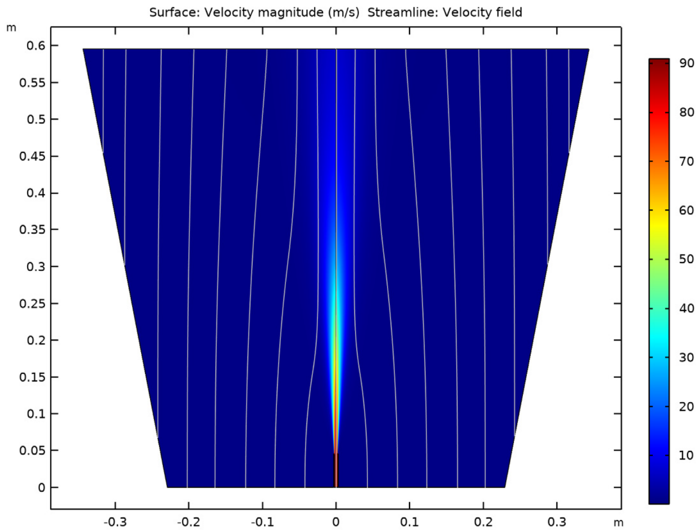


Figure 1: The velocity magnitude and flow paths (streamlines) of the reacting jet.

The temperature in the jet is shown in Figure 2 where a revolved dataset has been used to emphasize the structure of the round jet. The maximum temperature in the jet is seen to be approximately 2040 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 coflow 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.

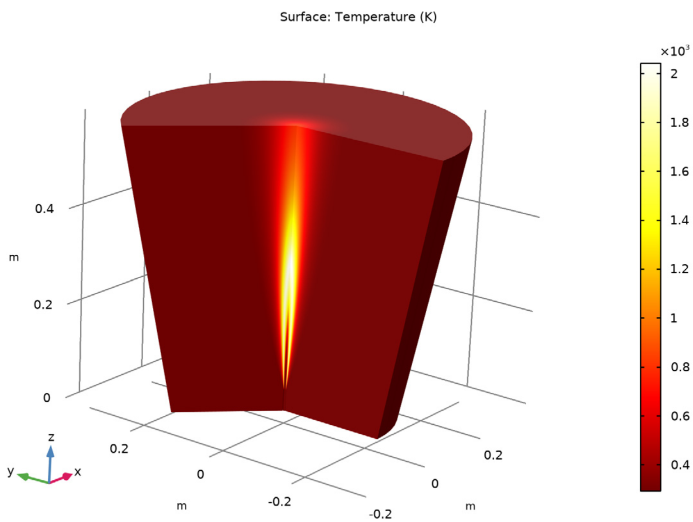


Figure 2: Jet temperature shown using a revolved dataset.

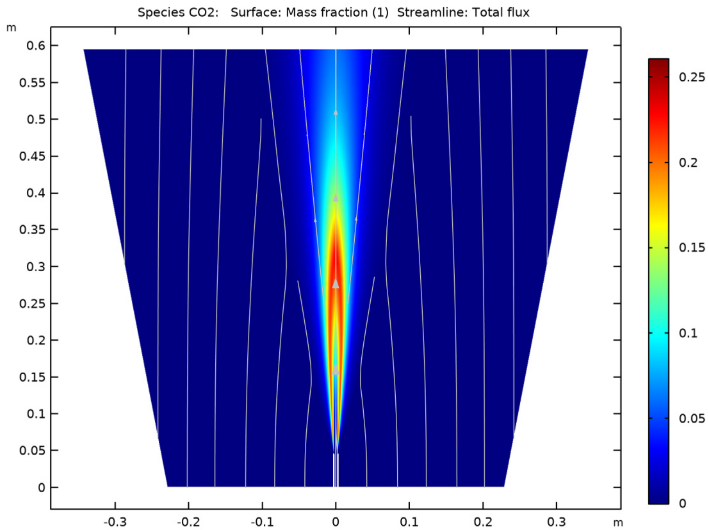


Figure 3: CO_2 mass fraction in the reacting jet.

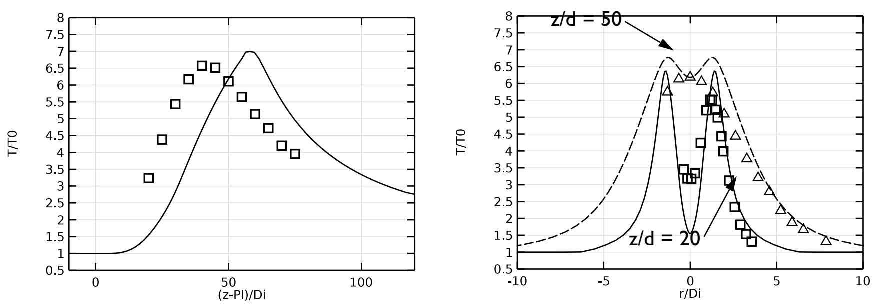


Figure 4: Jet temperature along the centerline (left), and radially at two different positions downstream of the pipe exit (right) scaled by the inlet temperature. The centerline and radial distance is scaled by the inner diameter of the pipe. Model results are plotted using lines, while experimental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

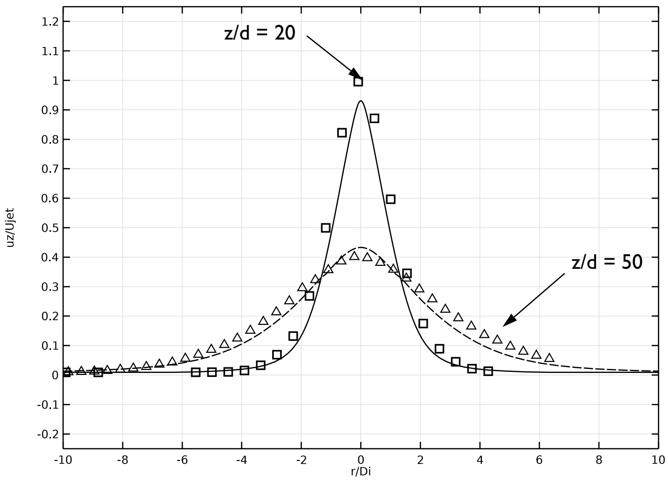


Figure 5: Axial velocity at two different positions downstream of the pipe exit, scaled by the inlet velocity. The radial distance is scaled by the inner diameter of the pipe. Model results are plotted using lines, while experimental results are indicated using symbols.

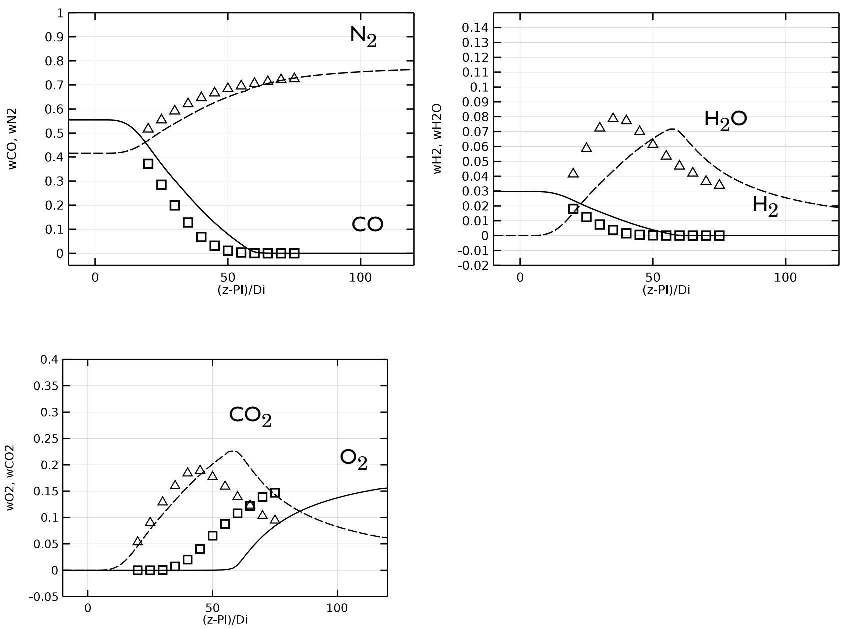


Figure 6: Species mass fractions along the jet centerline. The centerline distance is scaled by the

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

References

1. A. Cuoci, A. Frassoldati, G. Buzzi Ferraris, T. Faravelli, E. Ranzi, “The ignition, combustion and flame structure of carbon monoxide/hydrogen mixtures. Note 2: Fluid dynamics and kinetic aspects of syngas combustion,” *Int. J. Hydrogen Energy*, vol. 32, pp. 3486–3500, 2007

2. R.S. Barlow, G.J. Fiechtner, C.D. Carter, and J.-Y. Chen, “Experiments on the Scalar Structure of Turbulent CO/H2/N2 Jet Flames,” *Comb. and Flame*, vol. 120, pp. 549–569, 2000.

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

4. R.S. Barlow and others, “Sandia/ETH-Zurich CO/H2/N2 Flame Data - Release 1.1, ” http://www.sandia.gov/TNF/DataArch/SANDchnWeb/SANDchnDoc11.pdf, 2002.

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 **Blank Model**.

GLOBAL DEFINITIONS

Parameters 1

1 In the **Model Builder** window, under **Global Definitions** click **Parameters 1**.
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`.

ADD COMPONENT

In the **Home** toolbar, click **Add Component** and choose **2D Axisymmetric**.

ADD PHYSICS

1 In 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 Click to expand the **Dependent Variables** section. In the **Number of species** text field, type 6.
5 In the **Mass fractions** table, enter the following settings:

wCO
wO2
wCO2
wH2
wH2O
wN2

6 Click **Add to Component 1** in the window toolbar.
7 In the tree, select **Heat Transfer>Heat Transfer in Fluids (ht)**.
8 Click **Add to Component 1** in the window toolbar.
9 In the **Home** toolbar, click **Add Physics** to close the **Add Physics** window.

ADD MULTIPHYSICS

1 In the **Home** toolbar, click **Add Multiphysics** to open the **Add Multiphysics** window.
2 Go to the **Add Multiphysics** window.
3 In the tree, select **No Predefined Multiphysics Available for the Selected Physics Interfaces**.

4 Find the **Select the physics interfaces you want to couple** subsection. In the table, clear the **Couple** check box for **Transport of Concentrated Species (tcs)**.

5 In the tree, select **Fluid Flow>Nonisothermal Flow>Turbulent Flow>Turbulent Flow, k-ω**.

6 Click **Add to Component** in the window toolbar.

7 In the **Home** toolbar, click **Add Multiphysics** to close the **Add Multiphysics** window.

MULTIPHYSICS

Nonisothermal Flow 1 (nitf1)

1 In the **Settings** window for **Nonisothermal Flow**, locate the **Material Properties** section.

2 From the **Specify density** list, choose **Custom**.

3 From the ρ list, choose **Density (tcs/cdm1)**.

ADD STUDY

1 In 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 **General Studies>Stationary**.

4 Click **Add Study** in the window toolbar.

5 In the **Home** toolbar, click **Add Study** to close the **Add Study** window.

DEFINITIONS

Variables 1

1 In the **Home** toolbar, click a= **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 1

Rectangle 1 (r1)

1 In the **Geometry** toolbar, click **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 Click **Build Selected**.

Rectangle 2 (r2)

1 In the **Geometry** toolbar, click **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 `Pl`.

5 Locate the **Position** section. In the **r** text field, type `Di/2`.

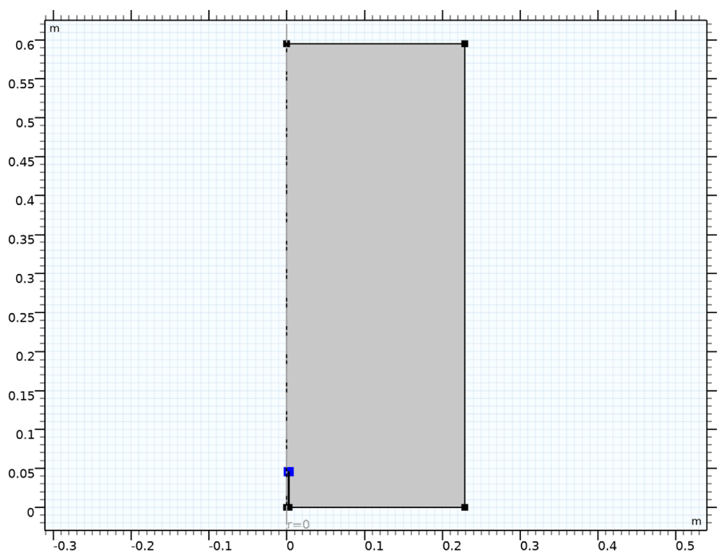
6 Click **Build Selected**.

Chamfer 1 (cha1)

1 In the **Geometry** toolbar, click **Chamfer**.

2 On the object **r2**, select Points 3 and 4 only.

It might be easier to select the points by using the **Selection List** window. To open this window, in the **Home** toolbar click **Windows** and choose **Selection List**. (If you are running the cross-platform desktop, you find **Windows** in the main menu.)



3 In the **Settings** window for **Chamfer**, locate the **Distance** section.

4 In the **Distance from vertex** text field, type `Pth*0.15`.

5 Click **Build Selected**.

6 Click the **Zoom Extents** button in the **Graphics** toolbar.

Polygon 1 (pol1)

1 In the **Geometry** toolbar, click **Polygon**.

2 In the **Settings** window for **Polygon**, locate the **Coordinates** section.

3 From the **Data source** list, choose **Vectors**.

4 In the **r** text field, type `GeomW GeomW*1.5 GeomW*1.5 GeomW`.

5 In the **z** text field, type `0 GeomH GeomH GeomH`.

6 Click **Build Selected**.

Union 1 (uni1)

1 In the **Geometry** toolbar, click **Booleans and Partitions** and choose **Union**.

2 Select the objects **pol1** and **r1** only.

3 In the **Settings** window for **Union**, locate the **Union** section.

4 Clear the **Keep interior boundaries** check box.

5 Click **Build Selected**.

Difference 1 (dif1)

1 In the **Geometry** toolbar, click **Booleans and Partitions** and choose **Difference**.

2 Select the object **uni1** only.

3 In the **Settings** window for **Difference**, locate the **Difference** section.

4 Find the **Objects to subtract** subsection. Select the **Activate Selection** toggle button.

5 Select the object **cha1** only.

6 Click **Build Selected**.

Line Segment 1 (ls1)

1 In the **Geometry** toolbar, click **More Primitives** and choose **Line Segment**.

2 In the **Settings** window for **Line Segment**, locate the **Starting Point** section.

3 From the **Specify** list, choose **Coordinates**.

4 Locate the **Endpoint** section. From the **Specify** list, choose **Coordinates**.

5 In the **r** text field, type `Di/2`.

6 Locate the **Starting Point** section. In the **z** text field, type `Pl-0.15*Pth`.

7 Locate the **Endpoint** section. In the **z** text field, type `Pl-0.15*Pth`.

8 Click **Build Selected**.

Line Segment 2 (ls2)

1 In the **Geometry** toolbar, click **More Primitives** and choose **Line Segment**.

2 In the **Settings** window for **Line Segment**, locate the **Starting Point** section.

3 From the **Specify** list, choose **Coordinates**.

4 Locate the **Endpoint** section. From the **Specify** list, choose **Coordinates**.

5 Locate the **Starting Point** section. In the **r** text field, type `Di/2+Pth`.

6 Locate the **Endpoint** section. In the **r** text field, type `GeomW+0.5*(Pl-0.15*Pth)*GeomW/GeomH`.

7 Locate the **Starting Point** section. In the **z** text field, type `Pl-0.15*Pth`.

8 Locate the **Endpoint** section. In the **z** text field, type `Pl-0.15*Pth`.

9 Click **Build Selected**.

Line Segment 3 (ls3)

1 In the **Geometry** toolbar, click **More Primitives** and choose **Line Segment**.

2 In the **Settings** window for **Line Segment**, locate the **Starting Point** section.

3 From the **Specify** list, choose **Coordinates**.

4 Locate the **Endpoint** section. From the **Specify** list, choose **Coordinates**.

5 Locate the **Starting Point** section. In the **r** text field, type `Di/2`.

6 Locate the **Endpoint** section. In the **r** text field, type `Di/2+(GeomH-Pl+Pth*0.15)*tan(pi/180)`.

7 Locate the **Starting Point** section. In the **z** text field, type `Pl-0.15*Pth`.

8 Locate the **Endpoint** section. In the **z** text field, type `GeomH`.

9 Click **Build Selected**.

Line Segment 4 (ls4)

1 In the **Geometry** toolbar, click **More Primitives** and choose **Line Segment**.

2 In the **Settings** window for **Line Segment**, locate the **Starting Point** section.

3 From the **Specify** list, choose **Coordinates**.

4 Locate the **Endpoint** section. From the **Specify** list, choose **Coordinates**.

5 Locate the **Starting Point** section. In the **r** text field, type `Di/2+Pth`.

6 Locate the **Endpoint** section. In the **r** text field, type `Di/2+Pth+(GeomH-Pl+Pth*0.15)*tan(5*pi/180)`.

7 Locate the **Starting Point** section. In the **z** text field, type `Pl-0.15*Pth`.

8 Locate the **Endpoint** section. In the **z** text field, type `GeomH`.

9 Click **Build Selected**.

Form Union (fin)

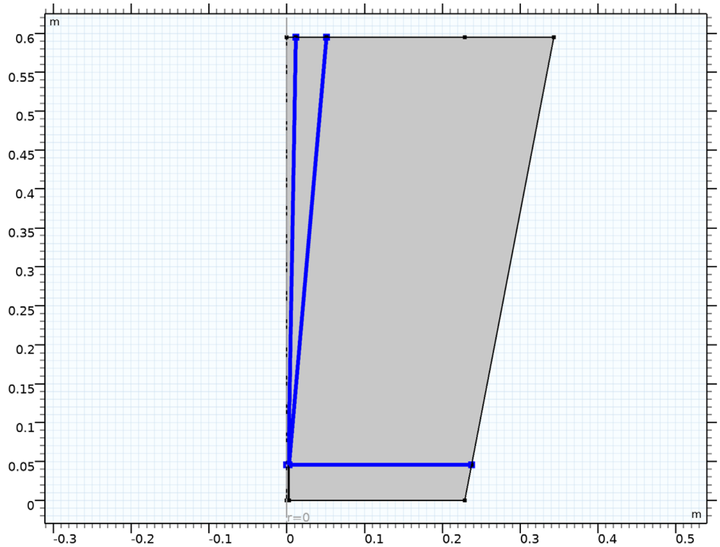
1 In the **Model Builder** window, click **Form Union (fin)**.

2 In the **Settings** window for **Form Union/Assembly**, click **Build Selected**.

Mesh Control Edges 1 (mce1)

1 In the **Geometry** toolbar, click **Virtual Operations** and choose **Mesh Control Edges**.

2 On the object **fin**, select Boundaries 4, 8, 13, and 14 only.



3 In the **Settings** window for **Mesh Control Edges**, click **Build Selected**.

4 Click the **Zoom Extents** button in the **Graphics** toolbar.

Form Composite Edges 1 (cme1)

1 In the **Geometry** toolbar, click **Virtual Operations** and choose **Form Composite Edges**.

2 On the object **mce1**, select Boundaries 3 and 11 only.

3 In the **Settings** window for **Form Composite Edges**, click **Build Selected**.

TURBULENT FLOW, K-ω (SPF)

Fluid Properties 1

1 In the **Model Builder** window, under **Component 1 (comp1)>Turbulent Flow, k-ω (spf)** click **Fluid Properties 1**.

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

1 In the **Physics** toolbar, click **Boundaries** and choose **Inlet**.

2 Select Boundary 2 only.

3 In the **Settings** window for **Inlet**, locate the **Boundary Condition** section.

4 From the list, choose **Fully developed flow**.

Inlet 2

In the **Physics** toolbar, click **Boundaries** and choose **Inlet**.

Inlet 1

1 In the **Model Builder** window, click **Inlet 1**.

2 In the **Settings** window for **Inlet**, locate the **Fully Developed Flow** section.

3 In the U_{av} text field, type `Ujet`.

Inlet 2

1 In the **Model Builder** window, click **Inlet 2**.

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 $\mathbf{u}_0$ vector as

0	r
Ucf	z

6 Locate the **Turbulence Conditions** section. From the I_T list, choose **Low (0.01)**.

7 From the L_T list, choose **User defined**.

8 In the text field, type `0.1*Di`.

Outlet 1

1 In 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)

1 In the **Model Builder** window, under **Component 1 (comp1)** 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.

1 In the **Model Builder** window, under **Component 1 (comp1)> Transport of Concentrated Species (tcs)** click **Transport Properties 1**.

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_{wCO} text field, type `M_CO`.

5 In the M_{wO2} text field, type `M_O2`.

6 In the M_{wCO2} text field, type `M_CO2`.

7 In the M_{wH2} text field, type `M_H2`.

8 In the M_{wH2O} text field, type `M_H2O`.

9 In the M_{wN2} text field, type `M_N2`.

Initial Values 1

1 In the **Model Builder** window, click **Initial Values 1**.

2 In the **Settings** window for **Initial Values**, locate the **Initial Values** section.

3 In the $\omega_{0,\mathrm{wCO}}$ text field, type `0`.

4 In the $\omega_{0,\mathrm{wO2}}$ text field, type `wcf_O2`.

5 In the $\omega_{0,\mathrm{wCO2}}$ text field, type `0`.

6 In the $\omega_{0,\mathrm{wH2}}$ text field, type `0`.

7 In the $\omega_{0,\mathrm{wH2O}}$ text field, type `0`.

Inflow 1

1 In 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 $x_{0,\mathrm{wCO}}$ text field, type `x0_CO`.

6 In the $x_{0,\mathrm{wO2}}$ text field, type `x0_O2`.

7 In the $x_{0,\mathrm{wCO2}}$ text field, type `x0_CO2`.

8 In the $x_{0,\mathrm{wH2}}$ text field, type `x0_H2`.

9 In the $x_{0,\mathrm{wH2O}}$ text field, type `x0_H2O`.

Inflow 2

1 In 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 $\omega_{0,\mathrm{wCO}}$ text field, type `1e-5`.

5 In the $\omega_{0,\mathrm{wO2}}$ text field, type `wcf_O2`.

6 In the $\omega_{0,\mathrm{wCO2}}$ text field, type `1e-5`.

7 In the $\omega_{0,\mathrm{wH2}}$ text field, type `1e-5`.

8 In the $\omega_{0,\mathrm{wH2O}}$ text field, type `1e-5`.

Outflow 1

1 In the **Physics** toolbar, click **Boundaries** and choose **Outflow**.

2 Select Boundary 3 only.

Reaction 1

1 In the **Physics** toolbar, click **Domains** and choose **Reaction**.

2 Select Domain 1 only.

3 In the **Settings** window for **Reaction**, locate the **Reaction Rate** section.

4 In the ν_{wCO} text field, type `-1`.

5 In the ν_{wO2} text field, type `-0.5`.

6 In the ν_{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 **Eddy-dissipation**.

Regularization makes the reaction system much easier to converge.

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

Reaction 2

1 Right-click **Reaction 1** and choose **Duplicate**.

2 In the **Settings** window for **Reaction**, locate the **Reaction Rate** section.

3 In the ν_{wCO} text field, type `0`.

4 In the ν_{wCO2} text field, type `0`.

5 In the ν_{wH2} text field, type `-1`.

6 In the ν_{wH2O} text field, type `1`.

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

DEFINITIONS

Interpolation 1 (int1)

1 In the **Home** toolbar, click f(X) **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
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 (Cp_CO2)

1 Right-click **Interpolation 1 (int1)** and choose **Duplicate**.

2 In the **Settings** window for **Interpolation**, locate the **Definition** section.

3 In the **Function name** text field, type `Cp_CO2`.

4 In the table, enter the following settings:

t	f(t)
300	51.140

t	f(t)
1000	8.910
2000	12.993

Interpolation 3 (Cp_CO3)

1 Right-click **Interpolation 2 (Cp_CO2)** 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 (Cp_H3)

1 Right-click **Interpolation 3 (Cp_CO3)** and choose **Duplicate**.

2 In the **Settings** window for **Interpolation**, locate the **Definition** section.

3 In the **Function name** text field, type `Cp_H2O`.

4 In the table, enter the following settings:

t	f(t)
300	7.999
1000	9.875
2000	12.224

Interpolation 5 (Cp_H2O2)

1 Right-click **Interpolation 4 (Cp_H3)** 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 (Cp_N3)

1 Right-click **Interpolation 5 (Cp_H2O2)** and choose **Duplicate**.

2 In the **Settings** window for **Interpolation**, locate the **Definition** section.

3 In the **Function name** text field, type `Cp_O2`.

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 1

1 In the **Model Builder** window, click **Variables 1**.

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	tcs.wr_wCO*Cp_CO(T)/M_CO+ tcs.wr_wCO2*Cp_CO2(T)/M_CO2+ tcs.wr_wH2*Cp_H2(T)/M_H2+ tcs.wr_wH2O*Cp_H2O(T)/M_H2O+ tcs.wr_wN2*Cp_N2(T)/M_N2+ tcs.wr_wO2*Cp_O2(T)/M_O2	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_H2O-(dH_H2+0.5*dH_O2)	J/mol	Enthalpy change reaction 2

Now setup the heat transfer interface.

HEAT TRANSFER IN FLUIDS (HT)

Fluid 1

1 In the **Model Builder** window, under **Component 1 (comp1)>Heat Transfer in Fluids (ht)** click **Fluid 1**.

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`.

4 Locate the **Thermodynamics, Fluid** section. From the **Specify Cp or** γ list, choose **Ideal gas: heat capacity at constant pressure**.

5 From the C_p list, choose **User defined**. In the associated text field, type `Cp_mix`.

Initial Values 1

1 In the **Model Builder** window, click **Initial Values 1**.

2 In the **Settings** window for **Initial Values**, locate the **Initial Values** section.

3 In the T text field, type `T0`.

Inflow 1

1 In the **Physics** toolbar, click **Boundaries** and choose **Inflow**.

2 Select Boundaries 2, 9, and 10 only.

3 In the **Settings** window for **Inflow**, locate the **Upstream Properties** section.

4 In the T_{ustr} text field, type `T0`.

Outflow 1

1 In the **Physics** toolbar, click **Boundaries** and choose **Outflow**.

2 Select Boundary 3 only.

Heat Source 1

1 In the **Physics** toolbar, click **Domains** and choose **Heat Source**.

2 Select Domain 1 only.

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 1

Mapped 1

1 In the **Mesh** toolbar, click **Mapped**.

2 In the **Settings** window for **Mapped**, click to expand the **Control Entities** section.

3 Clear the **Smooth across removed control entities** check box.

Distribution 1

1 Right-click **Mapped 1** and choose **Distribution**.

2 Select Boundaries 2 and 15 only.

3 In the **Settings** window for **Distribution**, locate the **Distribution** section.

4 From the **Distribution type** list, choose **Predefined**.

5 In the **Number of elements** text field, type 20.

6 In the **Element ratio** text field, type 4.

7 From the **Growth formula** list, choose **Geometric sequence**.

Distribution 2

1 In the **Model Builder** window, right-click **Mapped 1** and choose **Distribution**.

2 Select Boundaries 11, 16, and 17 only.

3 In the **Settings** window for **Distribution**, locate the **Distribution** section.

4 From the **Distribution type** list, choose **Predefined**.

5 In the **Number of elements** text field, type 200.

6 In the **Element ratio** text field, type 250.

7 From the **Growth formula** list, choose **Geometric sequence**.

Distribution 3

1 Right-click **Mapped 1** and choose **Distribution**.

2 Select Boundaries 9 and 18 only.

3 In the **Settings** window for **Distribution**, locate the **Distribution** section.

4 From the **Distribution type** list, choose **Predefined**.

5 In the **Number of elements** text field, type 20.

6 In the **Element ratio** text field, type 400.

7 From the **Growth formula** list, choose **Geometric sequence**.

8 Select the **Reverse direction** check box.

Distribution 4

1 Right-click **Mapped 1** and choose **Distribution**.

2 Select Boundaries 1, 4, and 8 only.

3 In the **Settings** window for **Distribution**, locate the **Distribution** section.

4 From the **Distribution type** list, choose **Predefined**.

5 In the **Number of elements** text field, type 20.

6 In the **Element ratio** text field, type 200.

7 From the **Growth formula** list, choose **Geometric sequence**.

8 Select the **Reverse direction** check box.

Distribution 5

1 Right-click **Mapped 1** and choose **Distribution**.

2 Select Boundary 12 only.

3 In the **Settings** window for **Distribution**, locate the **Distribution** section.

4 From the **Distribution type** list, choose **Predefined**.

5 In the **Number of elements** text field, type 20.

6 In the **Element ratio** text field, type 8.

7 From the **Growth formula** list, choose **Geometric sequence**.

Distribution 6

1 Right-click **Mapped 1** and choose **Distribution**.

2 Select Boundaries 3 and 13 only.

3 In the **Settings** window for **Distribution**, locate the **Distribution** section.

4 From the **Distribution type** list, choose **Predefined**.

5 In the **Number of elements** text field, type 20.

6 In the **Element ratio** text field, type 4.

7 From the **Growth formula** list, choose **Geometric sequence**.

8 Click **Build All**.

STUDY 1

Solution 1 (sol1)

1 In the **Study** toolbar, click **Show Default Solver**.

2 In the **Model Builder** window, expand the **Solution 1 (sol1)** node.

3 In the **Model Builder** window, expand the **Study 1>Solver Configurations>Solution 1 (sol1)>Stationary Solver 1** node.

4 In the **Model Builder** window, under **Study 1>Solver Configurations>Solution 1 (sol1)>Stationary Solver 1** click **Segregated 1**.

5 In the **Settings** window for **Segregated**, locate the **General** section.

6 In the **PID controller - proportional** text field, type 0.65.

7 In the **PID controller - 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 1>Solver Configurations>Solution 1 (sol1)>Stationary Solver 1>Segregated 1** click **Velocity u, Pressure p**.

10 In the **Settings** window for **Segregated Step**, locate the **General** section.

11 Under **Variables**, click **Add**.

12 In the **Add** dialog box, in the **Variables** list, choose **Wall temperature, downside (comp1.nitf1.TWall_d)**, **Wall temperature, upside (comp1.nitf1.TWall_u)**, and **Temperature (comp1.T)**.

13 Click **OK**.

14 In the **Model Builder** window, under **Study 1>Solver Configurations>Solution 1 (sol1)>Stationary Solver 1>Segregated 1** click **Mass fractions**.

15 In the **Settings** window for **Segregated Step**, click to expand the **Method and Termination** section.

16 In the **Number of iterations** text field, type `2`.

17 In the **Damping factor** text field, type `0.4`.

18 In the **Model Builder** window, under **Study 1>Solver Configurations>Solution 1 (sol1)>Stationary Solver 1>Segregated 1** right-click **Temperature** and choose **Disable**.

Solution 1 (sol1)

1 In the **Model Builder** window, collapse the **Study 1>Solver Configurations>Solution 1 (sol1)** node.

2 In the **Model Builder** window, right-click **Solution 1 (sol1)** and choose **Compute**.

Now move on to postprocess the result from the nonisothermal jet. Start by creating a mirrored 2D dataset as well as a revolved 3D dataset.

RESULTS

Mirror 2D 1

In the **Results** toolbar, click **More Datasets** and choose **Mirror 2D**.

Cut Line 2D 1

1 In the **Results** toolbar, click **Cut Line 2D**.

2 In the **Settings** window for **Cut Line 2D**, locate the **Data** section.

3 From the **Dataset** list, choose **Mirror 2D 1**.

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 `Pl+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

1 In the **Results** toolbar, click **Cut Line 2D**.

2 In the **Settings** window for **Cut Line 2D**, locate the **Data** section.

3 From the **Dataset** list, choose **Mirror 2D 1**.

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 `Pl+50*Di`.

6 Locate the **Advanced** section. Find the **Space variable** subsection. In the **x** text field, type `r_mirr50`.

Now apply the mirror dataset to the existing plot groups.

Velocity (spf)

1 In the **Model Builder** window, click **Velocity (spf)**.

2 In the **Settings** window for **2D Plot Group**, locate the **Data** section.

3 From the **Dataset** list, choose **Mirror 2D 1**.

4 In the **Velocity (spf)** toolbar, click **Plot**.

Streamline 1

Right-click **Velocity (spf)** and choose **Streamline**.

Streamline 1

1 In the **Model Builder** window, expand the **Results>Velocity (spf)** node, then click **Streamline 1**.

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. Find the **Point style** subsection. From the **Color** list, choose **Gray**.

6 In the **Velocity (spf)** toolbar, click **Plot**.

7 Click the **Zoom Extents** button in the **Graphics** toolbar.

Pressure (spf)

1 In the **Model Builder** window, click **Pressure (spf)**.

2 In the **Settings** window for **2D Plot Group**, locate the **Data** section.

3 From the **Dataset** list, choose **Mirror 2D 1**.

4 In the **Pressure (spf)** toolbar, click **Plot**.

Wall Resolution (spf)

1 In the **Model Builder** window, click **Wall Resolution (spf)**.

2 In the **Settings** window for **2D Plot Group**, locate the **Data** section.

3 From the **Dataset** list, choose **Mirror 2D 1**.

4 In the **Wall Resolution (spf)** toolbar, click **Plot**.

Mass fraction, CO2

1 In the **Model Builder** window, right-click **Concentration, CO2 (tcs)** and choose **Duplicate**.

2 In the **Settings** window for **2D Plot Group**, type `Mass fraction, CO2` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Mirror 2D 1**.

4 Locate the **Plot Settings** section. From the **Color** list, choose **White**.

Surface 1

1 In the **Model Builder** window, expand the **Mass fraction, CO2** node, then click **Surface 1**.

2 In the **Settings** window for **Surface**, locate the **Expression** section.

3 In the **Expression** text field, type `wCO2`.

4 In the **Mass fraction, CO2** toolbar, click **Plot**.

5 Click the **Zoom Extents** button in the **Graphics** toolbar.

Temperature, 3D (ht)

1 In the **Model Builder** window, click **Temperature, 3D (ht)**.

2 In the **Settings** window for **3D Plot Group**, locate the **Plot Settings** section.

3 Clear the **Plot dataset edges** check box.

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

Centerline data

1 In the **Results** toolbar, click **Table**.

2 In the **Settings** window for **Table**, type `Centerline data` in the **Label** text field.

3 Locate the **Data** section. Click **Import**.

4 Browse to the model's Application Libraries folder and double-click the file `round_jet_burner_chnAclY.fav`.

z/Di = 20, Radial Data

1 In the **Results** toolbar, click **Table**.

2 In the **Settings** window for **Table**, type `z/Di = 20, Radial Data` in the **Label** text field.

3 Locate the **Data** section. Click **Import**.

4 Browse to the model's Application Libraries folder and double-click the file `round_jet_burner_chnAd20Y.fav`.

z/Di = 50, Radial Data

1 In the **Results** toolbar, click **Table**.

2 In the **Settings** window for **Table**, type `z/Di = 50, Radial Data` in the **Label** text field.

3 Locate the **Data** section. Click **Import**.

4 Browse to the model's Application Libraries folder and double-click the file `round_jet_burner_chnAd50Y.fav`.

z/Di = 20, Radial Velocity Data

1 In the **Results** toolbar, click **Table**.

2 In the **Settings** window for **Table**, type `z/Di = 20, Radial Velocity Data` in the **Label** text field.

3 Locate the **Data** section. Click **Import**.

4 Browse to the model's Application Libraries folder and double-click the file `round_jet_burner_seq1420.dat`.

z/Di = 50, Radial Velocity Data

1 In the **Results** toolbar, click **Table**.

2 In the **Settings** window for **Table**, type `z/Di = 50, Radial Velocity Data` in the **Label** text field.

3 Locate the **Data** section. Click **Import**.

4 Browse to the model's Application Libraries folder and double-click the file `round_jet_burner_seq1450.dat`.

1D Plot Group 20

In the **Results** toolbar, click **1D Plot Group**.

Line Graph 1

1 Right-click **1D Plot Group 20** 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-Pl)/Di`.

7 Click to expand 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**.

10 In the table, enter the following settings:

Legends
`Model`

Table Graph 1

1 In the **Model Builder** window, right-click **1D Plot Group 20** 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**.

11 From the **Color** list, choose **Black**.

12 Find the **Line markers** subsection. From the **Marker** list, choose **Square**.

13 From the **Positioning** list, choose **In data points**.

14 Click to expand the **Legends** section. Select the **Show legends** check box.

15 From the **Legends** list, choose **Manual**.

16 In the table, enter the following settings:

Legends
`Exp.`

T @ centerline

1 In the **Model Builder** window, under **Results** click **1D Plot Group 20**.

2 In the **Settings** window for **1D Plot Group**, type `T @ centerline` in the **Label** text field.

3 Locate the **Plot Settings** section. Select the **x-axis label** check box.

4 In the associated text field, type `(z-Pl)/Di`.

5 Select the **y-axis label** check box.

6 In the associated text field, type `T/T0`.

7 Locate the **Axis** section. Select the **Manual axis limits** check box.

8 In the **x minimum** text field, type `-10`.

9 In the **x maximum** text field, type `120`.

10 In the **y minimum** text field, type `0.5`.

11 In the **y maximum** text field, type `8`.

12 Click to expand the **Title** section. From the **Title type** list, choose **Manual**.

13 In the **Title** text area, type `Temperature along the centerline`.

14 In the **T @ centerline** toolbar, click **Plot**.

1D Plot Group 21

1 In the **Home** toolbar, click **Add Plot Group** and choose **1D Plot Group**.

2 In the **Settings** window for **1D Plot Group**, locate the **Data** section.

3 From the **Dataset** list, choose **None**.

Line Graph 1

1 Right-click **1D Plot Group 21** and choose **Line Graph**.

2 In the **Settings** window for **Line Graph**, locate the **Data** section.

3 From the **Dataset** list, choose **Cut Line 2D 1**.

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 Locate the **Coloring and Style** section. From the **Color** list, choose **Black**.

8 Locate the **Legends** section. Select the **Show legends** check box.

9 From the **Legends** list, choose **Manual**.

10 In the table, enter the following settings:

Legends
z/Di = 20, Model

Line Graph 2

1 Right-click **Line Graph 1** and choose **Duplicate**.

2 In the **Settings** window for **Line Graph**, locate the **Data** section.

3 From the **Dataset** 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 In the **1D Plot Group 21** toolbar, click **Plot**.

Table Graph 1

1 In the **Model Builder** window, right-click **1D Plot Group 21** 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 Locate 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**.

10 In the **Scaling** text field, type `1/T0`.

11 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**.

17 In the table, enter the following settings:

Legends
`z/Di = 20, Exp`

Table Graph 2

1 Right-click **Table Graph 1** 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`

T @ z/Di = 20, 50

1 In the **Model Builder** window, under **Results** click **1D Plot Group 21**.
2 In the **Settings** window for **1D Plot Group**, type `T @ z/Di = 20, 50` in the **Label** text field.
3 Locate the **Title** section. From the **Title type** list, choose **Manual**.
4 In the **Title** text area, type `Temperature downstream of the pipe exit`.
5 Locate the **Plot Settings** section. Select the **x-axis label** check box.
6 In the associated text field, type `r/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.
10 In the **x minimum** text field, type `-10`.
11 In the **x maximum** text field, type `10`.
12 In the **y minimum** text field, type `0.5`.
13 In the **y maximum** text field, type `8`.
14 In the **T @ z/Di = 20, 50** toolbar, click **Plot**.

uz @ z/Di = 20, 50

1 In the **Model Builder** window, right-click **T @ z/Di = 20, 50** and choose **Duplicate**.
2 In the **Settings** window for **1D Plot Group**, type `uz @ z/Di = 20, 50` in the **Label** text field.

Line Graph 1

1 In the **Model Builder** window, expand the **uz @ z/Di = 20, 50** node, then click **Line Graph 1**.

2 In the **Settings** window for **Line Graph**, locate the **y-Axis Data** section.

3 In the **Expression** text field, type `w/Ujet`.

Line Graph 2

1 In the **Model Builder** window, 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 `w/Ujet`.

Table Graph 1

1 In the **Model Builder** window, click **Table Graph 1**.

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. In the **Scaling** text field, type `1/Ujet`.

Table Graph 2

1 In the **Model Builder** window, 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. In the **Scaling** text field, type `1/Ujet`.

uz @ z/Di = 20, 50

1 In the **Model Builder** window, click **uz @ z/Di = 20, 50**.

2 In the **Settings** window for **1D 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 **y minimum** text field, type `-0.25`.

6 In the **y maximum** text field, type `1.25`.

7 In the **uz @ z/Di = 20, 50** toolbar, click **Plot**.

8 Locate the **Title** section. From the **Title type** list, choose **None**.

CO, N2 @ centerline

1 In the **Model Builder** window, right-click **T @ centerline** and choose **Duplicate**.
2 In the **Settings** window for **1D Plot Group**, type `CO, N2 @ centerline` in the **Label** text field.
3 Locate the **Title** section. In the **Title** text area, type `Mass fraction along the centerline`.
4 Locate the **Plot Settings** section. In the **y-axis label** text field, type `wCO, wN2`.
5 Locate the **Axis** section. In the **y minimum** text field, type `-0.05`.
6 In the **y maximum** text field, type `1`.
7 In the **CO, N2 @ centerline** toolbar, click **Plot**.
8 Locate the **Legend** section. From the **Position** list, choose **Middle right**.

Line Graph 1

1 In the **Model Builder** window, expand the **CO, N2 @ centerline** node, then click **Line Graph 1**.
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

1 In the **Model Builder** window, click **Table Graph 1**.
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 In the **CO, N2 @ centerline** toolbar, click **Plot**.

Line Graph 2

1 In the **Model Builder** window, under **Results>CO, N2 @ centerline** right-click **Line Graph 1** 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 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

1 In the **Model Builder** window, under **Results>CO, N2 @ centerline** right-click **Table Graph 1** 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 In the **CO, N2 @ centerline** toolbar, click **Plot**.

H2, H2O @ centerline

1 In the **Model Builder** window, right-click **CO, N2 @ centerline** and choose **Duplicate**.

2 In the **Settings** window for **1D Plot Group**, type H2, H2O @ centerline in the **Label** text field.

Line Graph 1

1 In the **Model Builder** window, expand the **H2, H2O @ centerline** node, then click **Line Graph 1**.

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

1 In the **Model Builder** window, click **Table Graph 1**.

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

1 In the **Model Builder** window, 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 wH2O.

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

Legends
H2O, Model

Table Graph 2

1 In the **Model Builder** window, click **Table Graph 2**.

2 In the **Settings** window for **Table Graph**, locate the **Data** section.

3 In the **Columns** list, select **YH2O**.

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

Legends
H2O, Exp

H2, H2O @ centerline

1 In the **Model Builder** window, click **H2, H2O @ centerline**.

2 In the **Settings** window for **1D Plot Group**, locate the **Plot Settings** section.

3 In the **y-axis label** text field, type wH2, wH2O.

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 In the **H2, H2O @ centerline** toolbar, click **Plot**.

O2, CO2 @ centerline

1 In the **Model Builder** window, right-click **H2, H2O @ centerline** and choose **Duplicate**.

2 In the **Settings** window for **1D Plot Group**, type `O2, CO2 @ centerline` in the **Label** text field.

Line Graph 1

1 In the **Model Builder** window, expand the **O2, CO2 @ centerline** node, then click **Line Graph 1**.

2 In the **Settings** window for **Line Graph**, locate the **y-Axis Data** section.

3 In the **Expression** text field, type `wO2`.

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

Legends
O2, Model

Table Graph 1

1 In the **Model Builder** window, click **Table Graph 1**.

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
O2, Exp.

Line Graph 2

1 In the **Model Builder** window, 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

1 In the **Model Builder** window, 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`

O2, CO2 @ centerline

1 In the **Model Builder** window, click **O2, CO2 @ centerline**.

2 In the **Settings** window for **1D Plot Group**, locate the **Plot Settings** section.

3 In the **y-axis label** text field, type `wO2, wCO2`.

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 In the **O2, CO2 @ centerline** toolbar, click **Plot**.