Created in COMSOL Multiphysics 6.1

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·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:

$$\mathrm{Da} = \frac{\tau_\mathrm{T}}{\tau_\mathrm{c}} \ll 1$$

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

$$r_{\mathrm{ED},j} = \frac{\alpha_j}{\tau_\mathrm{T}}\rho \cdot \min\left[\min\left(\frac{\omega_r}{\nu_{\mathrm{r}j} M_\mathrm{r}}\right), \beta \sum_\mathrm{p} \left(\frac{\omega_\mathrm{p}}{\nu_{\mathrm{p}j} M_\mathrm{p}}\right)\right] \quad (2)$$

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 nonpremixed 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.

THERMAL PROPERTIES — HEAT OF REACTION AND HEAT CAPACITY

In this model, a thermodynamic system including all present species is set up. The system is used to define species as well as mixture properties dependent on temperature and composition. When coupling the Chemistry interface to the Thermodynamic system, all thermodynamic and transport properties needed are automatically defined.

Two of the thermal properties needed are the heat of reaction and the heat capacity of the mixture. Figure 1 shows the variation of enthalpy of formation with temperature for all individual species. The enthalpy of formation is seen to increase with temperature for all species, and accurate results will be obtained by taking the temperature-dependence into consideration.

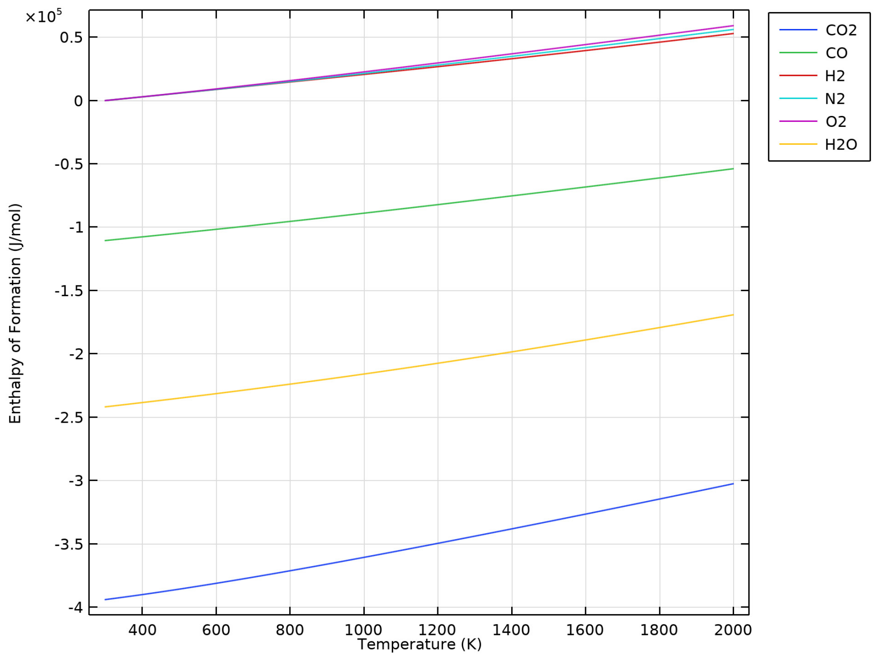


Figure 1: Enthalpy of formation for all individual species.

The heat capacities for all species in the system plotted against temperature are seen in Figure 2. As for the enthalpy of formation, all species' heat capacities increase with temperature, making it relevant to also take the temperature-dependence on heat capacity into consideration.

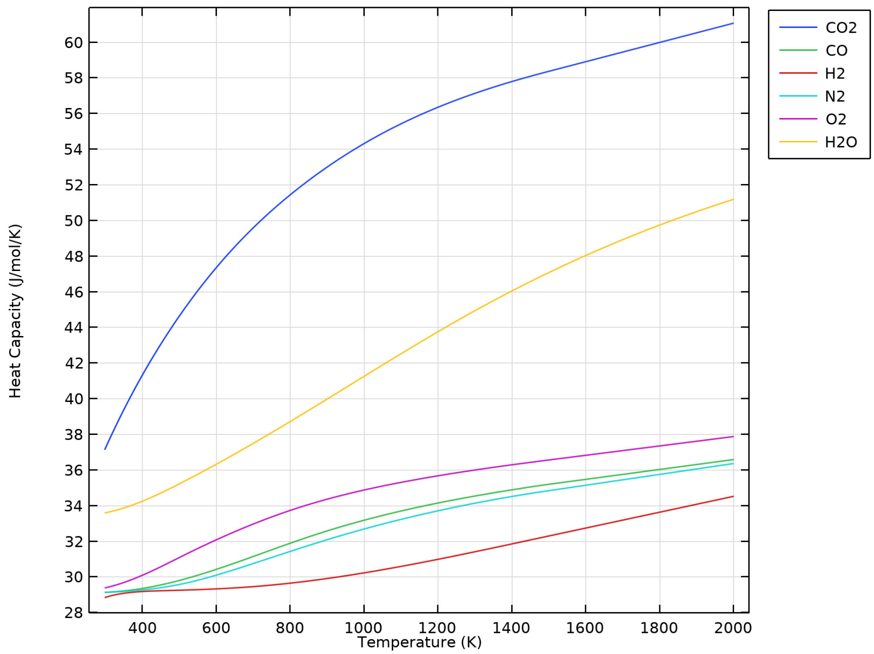


Figure 2: Heat capacity for all individual species.

The heat of formations for each species at $T = 298$ K are given in Table 1 and the heat capacities at $T = 300$ K and $T = 2000$ K are given in Table 2. Both tables compare data based on Ref. 6 and Ref. 7 to calculated values from COMSOL. By using these values in Equation 3, the heat of formation at $T = 298$ K can be calculated. Since the heat of formation of the products is lower than that of the reactants, both reactions are exothermic and release heat:

$$\Delta H_r = \sum_{\text{products}} \Delta H_{f,298\text{ K}} - \sum_{\text{reactants}} \Delta H_{f,298\text{ K}} \quad (3)$$

TABLE 1: SPECIES ENTHALPY OF FORMATION AT 298.15 K FROM BOTH REFERENCE DATA AND COMSOL.

SPECIES	ΔH_f (kJ/mol) T = 298.15 K (Ref. 6)	ΔH_f (kJ/mol) T = 298.15 K (COMSOL)
N_2	0	0
H_2	0	0
O_2	0	0
H_2O	-241.84	-241.82
CO	-110.54	-110.53
CO_2	-393.55	-393.98

TABLE 2: SPECIES HEAT CAPACITY AT 300 K AND 2000 K FROM BOTH REFERENCE DATA AND COMSOL.

SPECIES	C_p (J/mol/K) T = 300 K (Ref. 6, Ref. 7 for CO and CO2)	C_p (J/mol/K) T = 300 K (COMSOL)	C_p (J/mol/K) T = 2000 K (Ref. 6)	C_p (J/mol/K) T = 2000 K (COMSOL)
N_2	29.075	29.142	35.987	36.368
H_2	28.878	28.857	34.238	34.528
O_2	29.330	29.395	37.790	37.882
H_2O	33.468	33.602	51.145	51.193
CO	29.035	29.136	33.254	36.591
CO_2	37.101	37.225	54.363	61.078

Results and Discussion

The resulting velocity field in the nonisothermal reacting jet is visualized in Figure 3. 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.

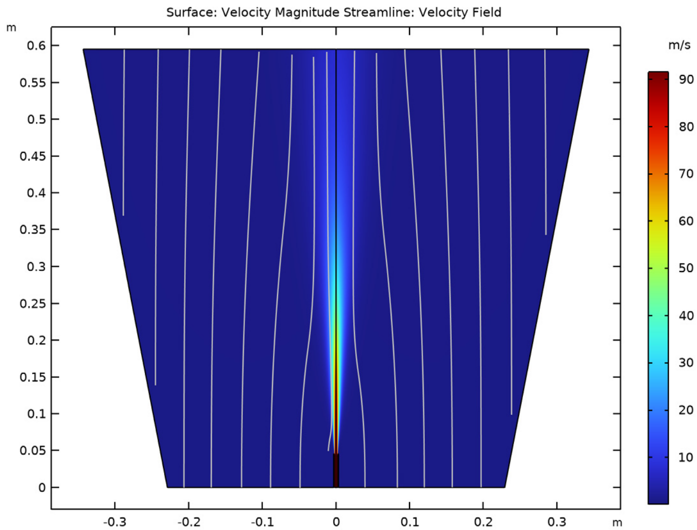


Figure 3: The velocity magnitude and flow paths (streamlines) of the reacting jet.

The temperature in the jet is shown in Figure 4 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 2150 K. The carbon dioxide mass fraction in the reacting jet is plotted in Figure 5. 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 4. This implies that there is no lift-off and the flame is attached to the pipe.

In Figure 6, Figure 7, and Figure 8 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 6 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 6 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 7, using the same down stream positions. The axial velocity is found to compare well with the experimental values at both positions.

In Figure 8 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.

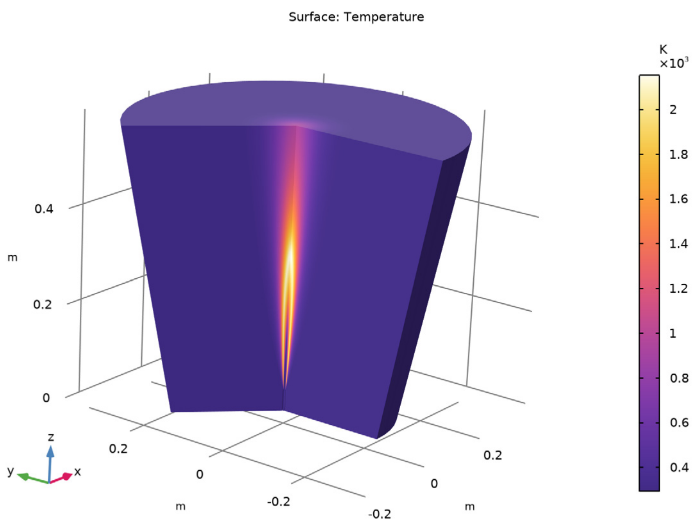


Figure 4: Jet temperature shown using a revolved dataset.

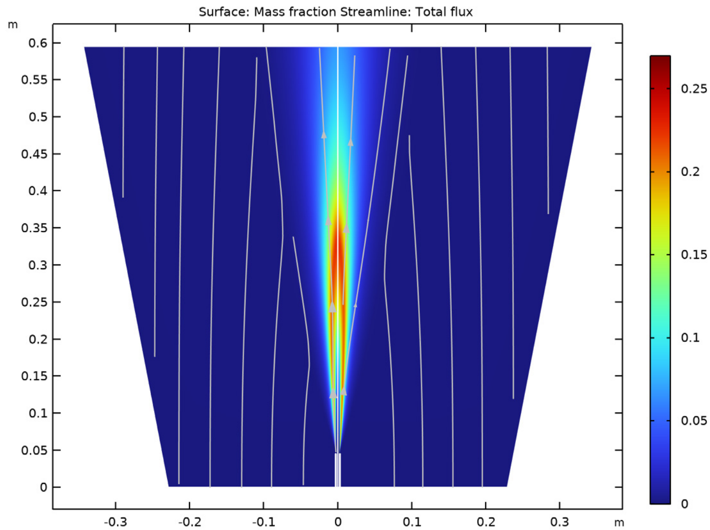


Figure 5: CO_2 mass fraction in the reacting jet.

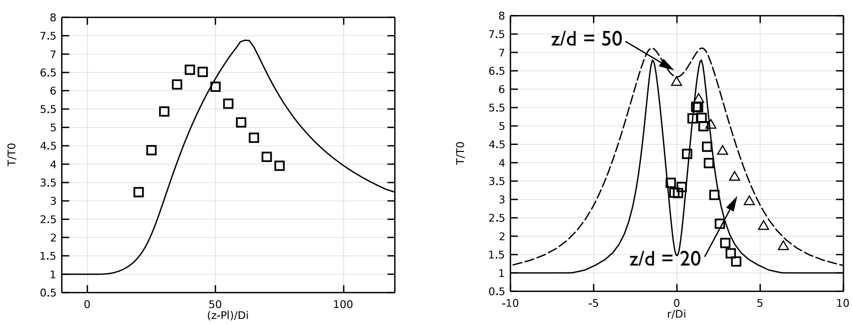


Figure 6: Jet temperature along the centerline (left), and radially at two different positions downstream of the pipe exit (right) scaled by the inlet temperature. The centerline and radial distance is scaled by the inner diameter of the pipe. Model results are plotted using lines, while experimental results are indicated using symbols. The downstream positions are defined in terms of the inner diameter of the pipe (d).

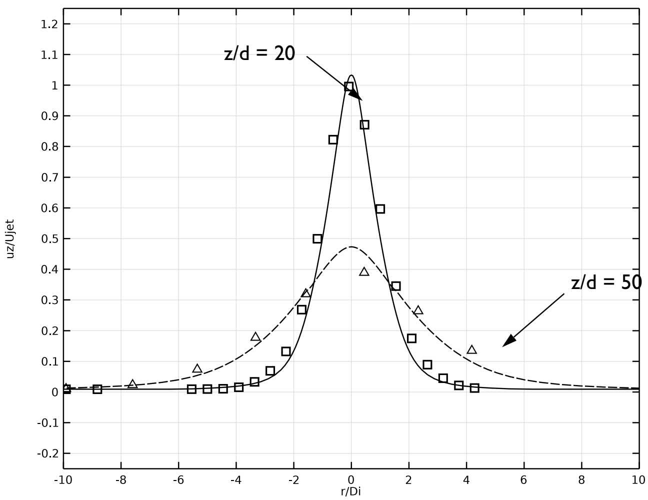


Figure 7: Axial velocity at two different positions downstream of the pipe exit, scaled by the inlet velocity. The radial distance is scaled by the inner diameter of the pipe. Model results are plotted using lines, while experimental results are indicated using symbols.

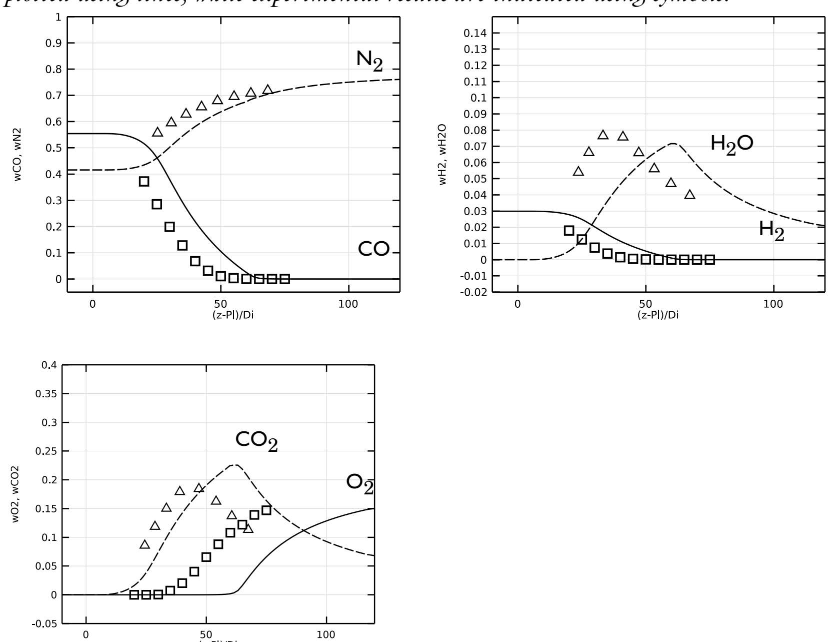


Figure 8: Species mass fractions along the jet centerline. The centerline distance is scaled by the

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, and 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 Mischungsstruktur 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., Pittsburgh, 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. Hydrog. Energy*, vol. 32, pp. 3471–3485, 2007.

7. B.E. Poling, J.M. Prausnitz, and J.P. O'Connell, *The Properties of Gases and Liquids,* McGraw-Hill, 2001.

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

1 In the **Model Wizard** window, click **2D Axisymmetric**.

2 In the **Select Physics** tree, select **Chemical Species Transport>Nonisothermal Reacting Flow>Turbulent Flow>Turbulent Flow, k-ω**.

3 Click **Add**.

4 In the **Added physics interfaces** tree, select **Transport of Concentrated Species (tcs)**.

5 In the **Number of species** text field, type `6`.

6 In the **Mass fractions** table, enter the following settings:

wCO
wO2
wCO2
wH2
wH2O
wN2

7 Click **Study**.

8 In the **Select Study** tree, select **General Studies>Stationary**.

9 Click **Done**.

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_parameters.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`.

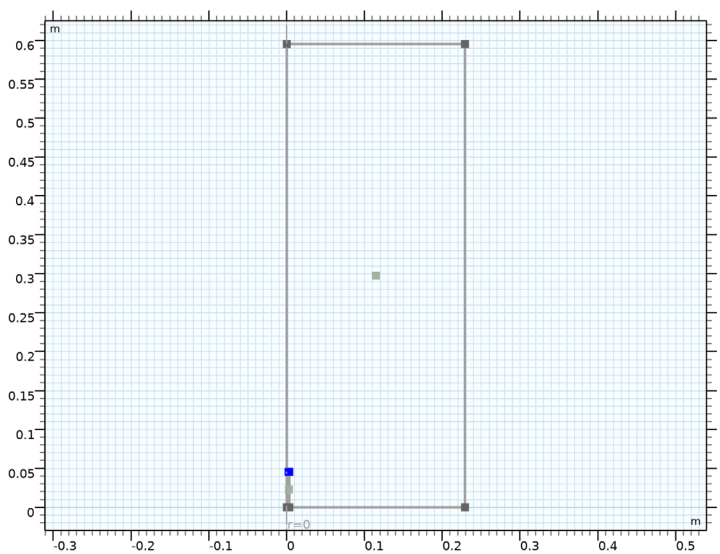
6 Click **Build Selected**.

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. Click to 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 In the **z** text field, type `Pl-0.15*Pth`.

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

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

7 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 In the **r** text field, type `Di/2+Pth`.

5 In the **z** text field, type `Pl-0.15*Pth`.

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

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

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

5 In the **z** text field, type `Pl-0.15*Pth`.

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

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

8 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 In the **r** text field, type `Di/2+Pth`.

5 In the **z** text field, type `Pl-0.15*Pth`.

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

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

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

9 Click **Build Selected**.

Form Union (fin)

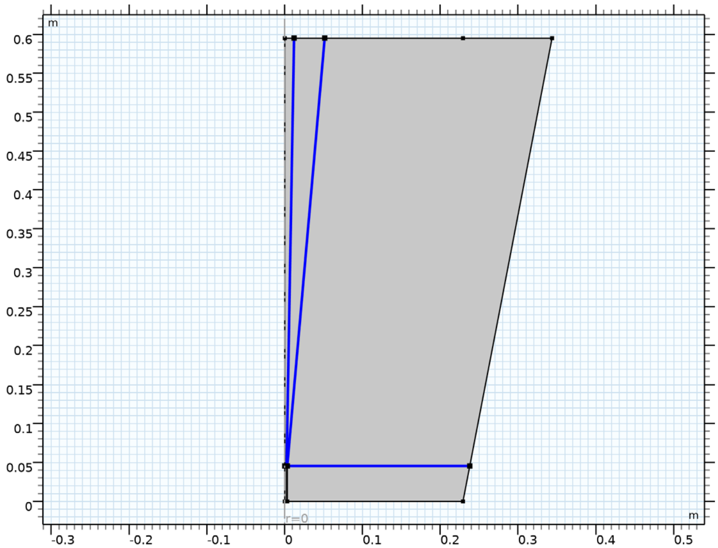
1 In the **Model Builder** window, click **Form Union (fin)**.

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**.

Define a **Thermodynamic System** that can be used for several physical properties in the model. The system is in gas phase and consists of water, hydrogen, oxygen, nitrogen, carbon monoxide and carbon dioxide.

GLOBAL DEFINITIONS

In the **Physics** toolbar, click **Thermodynamics** and choose **Thermodynamic System**.

SELECT SYSTEM

1 Go to the **Select System** window.

2 Click **Next** in the window toolbar.

SELECT SPECIES

1 Go to the **Select Species** window.

2 In the **Species** list, select **water (7732-18-5, H2O)**.

3 Click + **Add Selected**.

4 In the **Species** list, select **carbon monoxide (630-08-0, CO)**.

5 Click + **Add Selected**.

6 In the **Species** list, select **carbon dioxide (124-38-9, CO2)**.

7 Click + **Add Selected**.

8 In the **Species** list, select **nitrogen (7727-37-9, N2)**.

9 Click + **Add Selected**.

10 In the **Species** list, select **oxygen (7782-44-7, O2)**.

11 Click + **Add Selected**.

12 In the **Species** list, select **hydrogen (1333-74-0, H2)**.

13 Click + **Add Selected**.

14 Click **Next** in the window toolbar.

SELECT THERMODYNAMIC MODEL

1 Go to the **Select Thermodynamic Model** window.

2 Click **Finish** in the window toolbar.

GLOBAL DEFINITIONS

Gas System 1 (pp1)

As stated in the **Model Definition** section, the heat of reaction and heat capacity of the mixture are dependent on temperature and composition. To display their dependence, plots where the enthalpy of formation and heat capacity are plotted against a temperature span between 298.15 and 2000 K are later created. The functions necessary for these plots will now be obtained.

1 In the **Model Builder** window, under **Global Definitions>Thermodynamics** right-click **Gas System 1 (pp1)** and choose **Species Property**.

SELECT PROPERTIES

1 Go to the **Select Properties** window.
2 In the list, select **Heat capacity (Cp) (J/(K*mol))**.
3 Click **Add Selected**.
4 In the list, select **Enthalpy of formation (J/mol)**.
5 Click **Add Selected**.
6 Click **Next** in the window toolbar.

SELECT PHASE

1 Go to the **Select Phase** window.
2 Click **Next** in the window toolbar.

SELECT SPECIES

1 Go to the **Select Species** window.
2 Click **Add All**.
3 Click **Next** in the window toolbar.

SPECIES PROPERTY OVERVIEW

1 Go to the **Species Property Overview** window.
2 Click **Finish** in the window toolbar.

CHEMISTRY (CHEM)

Reaction 1

1 In the **Model Builder** window, under **Component 1 (comp1)** right-click **Chemistry (chem)** and choose **Reaction**.
2 In the **Settings** window for **Reaction**, locate the **Reaction Formula** section.
3 In the **Formula** text field, type `CO+O2=>CO2`.
4 Click **Apply**.

Since all species in the reaction are written using their chemical formulas, their molar masses are pre-defined to come from thermodynamics. Moreover, the reaction can also be balanced using the **Balance** button.

Click **Balance** in the upper-right corner of the **Reaction Formula** section.

Reaction 2

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

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

3 In the **Formula** text field, type `H2+O2=>H2O`.

4 Click **Apply**.

5 Click **Balance** in the upper-right corner of the **Reaction Formula** section.

Species 1

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

2 In the **Settings** window for **Species**, locate the **Name** section.

3 In the text field, type `N2`.

Since a **Thermodynamic system** is defined earlier, the **Thermodynamics** check box can be selected that uses the values for density and heat capacity from the system.

1 In the **Model Builder** window, click **Chemistry (chem)**.

2 In the **Settings** window for **Chemistry**, locate the **Mixture Properties** section.

3 Select the **Thermodynamics** check box.

4 Locate the **Species Matching** section. From the **Species solved for** list, choose **Transport of Concentrated Species**.

5 Find the **Bulk species** subsection. In the table, enter the following settings:

Species	Type	Mass fraction	Value (1)	From Thermodynamics
CO	Variable	wCO	Solved for	CO
CO2	Variable	wCO2	Solved for	CO2
H2	Variable	wH2	Solved for	H2
H2O	Variable	wH2O	Solved for	H2O
N2	Free species	wN2	Solved for	N2
O2	Variable	wO2	Solved for	O2

6 Click to expand the **Calculate Transport Properties** section. From the **Thermal conductivity** list, choose **User defined**.

7 In the k text field, type `k_mix`.

8 From the **Dynamic viscosity** list, choose **User defined**.

9 In the μ text field, type `mu_mix`.

TRANSPORT OF CONCENTRATED SPECIES (TCS)

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

Reaction 1

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

   Thanks to the balanced reactions, the stoichiometric coefficients are known.
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 `-2`.
5. In the ν_{wO2} text field, type `-1`.
6. In the ν_{wCO2} text field, type `2`.
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**.
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 `-2`.
6. In the ν_{wH2O} text field, type `2`.

The reaction rates are now decided and can be used for each reaction.

CHEMISTRY (CHEM)

1: 2 CO + O2 =2 CO2

1. In the **Model Builder** window, under **Component 1 (comp1)>Chemistry (chem)** click **1: 2 CO + O2 =2 CO2**.
2. In the **Settings** window for **Reaction**, locate the **Reaction Rate** section.
3. From the list, choose **User defined**.
4. In the r_j text field, type `tcs.treac1.r`.
5. Find the **Volumetric overall reaction order** subsection. In the **Forward** text field, type `0`.

2: 2 H2 + O2 =2 H2O

1 In the **Model Builder** window, click **2: 2 H2 + O2 =2 H2O**.

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

3 From the list, choose **User defined**.

4 In the r_j text field, type `tcs.treac2.r`.

5 Find the **Volumetric overall reaction order** subsection. In the **Forward** text field, type `0`.

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**.

Initial Values 1

1 In the **Model Builder** window, under **Component 1 (comp1)> Transport of Concentrated Species (tcs)** 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 $x_{0,\text{wH2O}}$ text field, type `x0_H2O`.

Inflow 2

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

2 In the **Settings** window for **Inflow**, locate the **Inflow** section.

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

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

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

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

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

8 Select Boundaries 9 and 10 only.

Outflow 1

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

2 Select Boundary 3 only.

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 **Model Input** section.

3 Click **Make All Model Inputs Editable** in the upper-right corner of the section.

4 Locate the **Fluid Properties** section. From the ρ list, choose **Density (chem)**.

5 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**.

5 Locate the **Fully Developed Flow** section. In the U_{av} text field, type `Ujet`.

Inlet 2

1 In 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 $\mathbf{u}_0$ 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.

HEAT TRANSFER IN FLUIDS (HT)

Initial Values 1

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

Fluid 1

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

2 In the **Settings** window for **Fluid**, locate the **Model Input** section.

3 Click **Make All Model Inputs Editable** in the upper-right corner of the section.

4 Locate the **Heat Convection** section. From the $\mathbf{u}$ list, choose **Velocity field (spf)**.

5 Locate the **Heat Conduction, Fluid** section. From the k list, choose **User defined**. In the associated text field, type `k_mix`.

6 Locate the **Thermodynamics, Fluid** section. From the ρ list, choose **Density (chem)**.

7 From the C_p list, choose **Heat capacity at constant pressure (chem)**.

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.

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 rate** list, choose **Exponential**.

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 rate** list, choose **Exponential**.

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 rate** list, choose **Exponential**.

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 rate** list, choose **Exponential**.

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 rate** list, choose **Exponential**.

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 rate** list, choose **Exponential**.

8 Click **Build All**.

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

STUDY 1

Solution 1 (sol1)

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

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

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

4 In the **PID controller - derivative** text field, type `0.025`.

5 In the **Target error estimate** text field, type `0.1`.

6 In the **Model Builder** window, expand the **Study 1>Solver Configurations>Solution 1 (sol1)>Stationary Solver 1>Segregated 1** node, then click **Velocity u, Pressure p**.

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

8 Under **Variables**, click **Add**.

9 In the **Add** dialog box, in the **Variables** list, choose **Wall temperature, downside (comp1.nirf1.TWall_d)**, **Wall temperature, upside (comp1.nirf1.TWall_u)**, and **Temperature (comp1.T)**.

10 Click **OK**.

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

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

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

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

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

GLOBAL DEFINITIONS

The enthalpy of formation and heat capacity plots will now be created (Figure 1 and Figure 2).

Gas System 1 (pp1)

In the **Model Builder** window, expand the **Global Definitions>Thermodynamics>Gas System 1 (pp1)>Mixture** node.

Enthalpy of formation 1 (EnthalpyF_carbon_dioxide_Gas12, EnthalpyF_carbon_dioxide_Gas12_Dtemperature, EnthalpyF_carbon_dioxide_Gas12_Dpressure)

1 In the **Model Builder** window, expand the **Global Definitions>Thermodynamics> Gas System 1 (pp1)>Mixture>Vapor** node, then click **Global Definitions>Thermodynamics> Gas System 1 (pp1)>carbon dioxide>Vapor> Enthalpy of formation 1 (EnthalpyF_carbon_dioxide_Gas12, EnthalpyF_carbon_dioxide_Gas12_Dtemperature, EnthalpyF_carbon_dioxide_Gas12_Dpressure)**.
2 In the **Settings** window for **Species Property**, click to expand the **Plot Parameters** section.
3 In the table, enter the following settings:

Argument	Lower limit	Upper limit
temperature	298.15	2000

4 Click **Create Plot**.

RESULTS

When working with the functions, they tend to load for a while. By choosing to manually save data in the model under **Results**, it will be possible to enable **Save plot data** under each plot group and therefore shorten the loading time.

1 In the **Settings** window for **Results**, locate the **Save Data in the Model** section.
2 From the **Save plot data** list, choose **Manual**.

Enthalpy of Formation

1 In the **Model Builder** window, under **Results** click **1D Plot Group 1**.
2 In the **Settings** window for **1D Plot Group**, type `Enthalpy of Formation` in the **Label** text field.
3 Locate the **Save Data in the Model** section. Select the **Save plot data** check box.
4 In a similar fashion, repeat the steps above, to create plots with the same temperature limits for the rest of the species.

1D Plot Group 2

In the **Model Builder** window, expand the **Results>1D Plot Group 2** node.

Function 1

In the **Model Builder** window, expand the **Results>Enthalpy of Formation** node, then click **Function 1**.

Function 2

1. Drag and drop below **Enthalpy of Formation Function 1**.
2. Drag-drop all functions into the same plot group to plot them in the same graph.

Since **1D Plot Group 2** - **1D Plot Group 6** are empty now, delete them.

1D Plot Group 2, 1D Plot Group 3, 1D Plot Group 4, 1D Plot Group 5, 1D Plot Group 6

1. In the **Model Builder** window, under **Results**, Ctrl-click to select **1D Plot Group 2**, **1D Plot Group 3**, **1D Plot Group 4**, **1D Plot Group 5**, and **1D Plot Group 6**.
2. Right-click and choose **Delete**.

The same procedure will now be performed for the heat capacity functions. As before, start by creating plots for each of the heat capacity functions.

GLOBAL DEFINITIONS

Heat capacity (Cp) 1 (HeatCapacityCp_carbon_dioxide_Gas11, HeatCapacityCp_carbon_dioxide_Gas11_Dtemperature, HeatCapacityCp_carbon_dioxide_Gas11_Dpressure)

1. In the **Model Builder** window, under **Global Definitions>Thermodynamics>Gas System 1 (pp1)>carbon dioxide>Vapor** click **Heat capacity (Cp) 1 (HeatCapacityCp_carbon_dioxide_Gas11, HeatCapacityCp_carbon_dioxide_Gas11_Dtemperature, HeatCapacityCp_carbon_dioxide_Gas11_Dpressure)**.
2. In the **Settings** window for **Species Property**, locate the **Plot Parameters** section.
3. In the table, enter the following settings:

Argument	Lower limit	Upper limit
temperature	298.15	2000

4. Click **Create Plot**.

RESULTS

Heat Capacity

1. In the **Settings** window for **1D Plot Group**, type `Heat Capacity` in the **Label** text field.
2. Locate the **Save Data in the Model** section. Select the **Save plot data** check box.
3. Repeat creating plots for the functions **Heat capacity (Cp) 2** - **Heat capacity (Cp) 6** using the same temperature limits.

1D Plot Group 3

In the **Model Builder** window, expand the **Results>1D Plot Group 3** node.

Function 1

In the **Model Builder** window, expand the **Results>Heat Capacity** node, then click **Function 1**.

Function 2

1 Drag and drop below **Heat Capacity** **Function 1**.
2 Repeat the drag-dropping of functions 3-6 into the **Heat Capacity** plot group.

1D Plot Group 3, 1D Plot Group 4, 1D Plot Group 5, 1D Plot Group 6, 1D Plot Group 7

Since **1D Plot Group 3** - **1D Plot Group 7** are empty now, delete them.

1 In the **Model Builder** window, under **Results**, Ctrl-click to select **1D Plot Group 3**, **1D Plot Group 4**, **1D Plot Group 5**, **1D Plot Group 6**, and **1D Plot Group 7**.
2 Right-click and choose **Delete**.

   Now we have two plots: one contains all enthalpy of formation functions, one contains all heat capacity functions.

Enthalpy of Formation

1 In the **Model Builder** window, under **Results** click **Enthalpy of Formation**.
2 In the **Settings** window for **1D Plot Group**, click to expand the **Title** section.
3 From the **Title type** list, choose **None**.
4 Locate the **Plot Settings** section.
5 Select the **x-axis label** check box. In the associated text field, type `Temperature (K)`.
6 Select the **y-axis label** check box. In the associated text field, type `Enthalpy of Formation (J/mol)`.
7 Locate the **Legend** section. From the **Layout** list, choose **Outside graph axis area**.

Function 1

1 In the **Model Builder** window, click **Function 1**.
2 In the **Settings** window for **Function**, click to expand the **Legends** section.
3 Select the **Show legends** check box.
4 From the **Legends** list, choose **Manual**.

5 In the table, enter the following settings:

Legends
CO2

Function 2

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

2 In the **Settings** window for **Function**, locate the **Legends** section.

3 Select the **Show legends** check box.

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

5 In the table, enter the following settings:

Legends
CO

Function 3

1 In the **Model Builder** window, click **Function 3**.

2 In the **Settings** window for **Function**, locate the **Legends** section.

3 Select the **Show legends** check box.

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

5 In the table, enter the following settings:

Legends
H2

Function 4

1 In the **Model Builder** window, click **Function 4**.

2 In the **Settings** window for **Function**, locate the **Legends** section.

3 Select the **Show legends** check box.

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

5 In the table, enter the following settings:

Legends
N2

Function 5

1 In the **Model Builder** window, click **Function 5**.

2 In the **Settings** window for **Function**, locate the **Legends** section.

3 Select the **Show legends** check box.

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

5 In the table, enter the following settings:

Legends
O2

Function 6

1 In the **Model Builder** window, click **Function 6**.

2 In the **Settings** window for **Function**, locate the **Legends** section.

3 Select the **Show legends** check box.

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

5 In the table, enter the following settings:

Legends
H2O

6 In the **Enthalpy of Formation** toolbar, click **Plot**.

Heat Capacity

All datasets **Grid 1D 1** - **Grid 1D 1k** contain the same information. Therefore, change the dataset to be the same as for the **Enthalpy of Formation** plot group.

1 In the **Model Builder** window, under **Results** click **Heat Capacity**.

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

3 From the **Dataset** list, choose **Grid 1D 1**.

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

5 Locate the **Plot Settings** section.

6 Select the **x-axis label** check box. In the associated text field, type `Temperature (K)`.

7 Select the **y-axis label** check box. In the associated text field, type `Heat Capacity (J/mol/K)`.

8 Locate the **Legend** section. From the **Layout** list, choose **Outside graph axis area**.

Function 1

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

2 In the **Settings** window for **Function**, locate the **Legends** section.

3 Select the **Show legends** check box.

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

5 In the table, enter the following settings:

Legends
CO2

Function 2

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

2 In the **Settings** window for **Function**, locate the **Legends** section.

3 Select the **Show legends** check box.

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

5 In the table, enter the following settings:

Legends
CO

Function 3

1 In the **Model Builder** window, click **Function 3**.

2 In the **Settings** window for **Function**, locate the **Legends** section.

3 Select the **Show legends** check box.

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

5 In the table, enter the following settings:

Legends
H2

Function 4

1 In the **Model Builder** window, click **Function 4**.

2 In the **Settings** window for **Function**, locate the **Legends** section.

3 Select the **Show legends** check box.

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

5 In the table, enter the following settings:

Legends
N2

Function 5

1 In the **Model Builder** window, click **Function 5**.

2 In the **Settings** window for **Function**, locate the **Legends** section.

3 Select the **Show legends** check box.

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

5 In the table, enter the following settings:

Legends
02

Function 6

1 In the **Model Builder** window, click **Function 6**.

2 In the **Settings** window for **Function**, locate the **Legends** section.

3 Select the **Show legends** check box.

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

5 In the table, enter the following settings:

Legends
H20

6 In the **Heat Capacity** toolbar, click **Plot**.

The datasets that are not used can now be deleted.

1 Delete all datasets **Grid 1D 1a** to **Grid 1D 1k**.

Now are the graphs for enthalpy of formation and heat capacity finished and are presented as Figure 1 and Figure 2 in the **Model Definition** section. To obtain the values presented in Table 1 and Table 2, **Evaluation Groups** are used, which gives the values for each function at the specific temperature.

Evaluation Group 1

1 In the **Results** toolbar, click **Evaluation Group**.

2 In the **Settings** window for **Evaluation Group**, locate the **Transformation** section.

3 Select the **Transpose** check box.

Enthalpy of Formation, 298 K

1 Right-click **Evaluation Group 1** and choose **Global Evaluation**.

2 In the **Settings** window for **Global Evaluation**, type `Enthalpy of Formation, 298 K` in the **Label** text field.

3 Locate the **Expressions** section. In the table, enter the following settings:

Expression	**Unit**	**Description**
EnthalpyF_carbon_dioxide_Gas12(298.15[K],1.0133E5[Pa])	J/mol	Enthalpy of formation 1
EnthalpyF_carbon_monoxide_Gas14(298.15[K],1.0133E5[Pa])	J/mol	Enthalpy of formation 2
EnthalpyF_hydrogen_Gas16(298.15[K],1.0133E5[Pa])	J/mol	Enthalpy of formation 3
EnthalpyF_nitrogen_Gas18(298.15[K],1.0133E5[Pa])	J/mol	Enthalpy of formation 4
EnthalpyF_oxygen_Gas110(298.15[K],1.0133E5[Pa])	J/mol	Enthalpy of formation 5
EnthalpyF_water_Gas112(298.15[K],1.0133E5[Pa])	J/mol	Enthalpy of formation 6

If clicking the **Evaluate** button now, no values will be given. This is because the datasets are empty. Using the feature **Get initial values** under **Study 1** enables evaluation of the function values in **Enthalpy of Formation, 298 K**.

STUDY 1

In the **Study** toolbar, click **Get Initial Value**.

RESULTS

Enthalpy of Formation, 298 K

1 In the **Model Builder** window, under **Results>Evaluation Group 1** click **Enthalpy of Formation, 298 K**.

2 In the **Evaluation Group 1** toolbar, click **Evaluate**.

Heat Capacity, 300 K

1 In the **Model Builder** window, right-click **Evaluation Group 1** and choose **Global Evaluation**.

2 In the **Settings** window for **Global Evaluation**, type `Heat Capacity, 300 K` in the **Label** text field.

3 Locate the **Expressions** section. In the table, enter the following settings:

Expression	Unit	Description
HeatCapacityCp_carbon_dioxide_Gas11(300[K], 1.0133E5[Pa])	J/(mol*K)	Heat capacity (Cp) 1
HeatCapacityCp_carbon_monoxide_Gas13(300[K], 1.0133E5[Pa])	J/(mol*K)	Heat capacity (Cp) 2
HeatCapacityCp_hydrogen_Gas15(300[K],1.0133E5[Pa])	J/(mol*K)	Heat capacity (Cp) 3
HeatCapacityCp_nitrogen_Gas17(300[K],1.0133E5[Pa])	J/(mol*K)	Heat capacity (Cp) 4
HeatCapacityCp_oxygen_Gas19(300[K],1.0133E5[Pa])	J/(mol*K)	Heat capacity (Cp) 5
HeatCapacityCp_water_Gas111(300[K],1.0133E5[Pa])	J/(mol*K)	Heat capacity (Cp) 6

4 In the **Evaluation Group 1** toolbar, click **=** **Evaluate**.

Heat Capacity, 2000 K

1 Right-click **Evaluation Group 1** and choose **Global Evaluation**.

2 In the **Settings** window for **Global Evaluation**, type `Heat Capacity, 2000 K` in the **Label** text field.

3 Locate the **Expressions** section. In the table, enter the following settings:

Expression	Unit	Description
HeatCapacityCp_carbon_dioxide_Gas11(2000[K], 1.0133E5[Pa])	J/(mol*K)	Heat capacity (Cp) 1
HeatCapacityCp_carbon_monoxide_Gas13(2000[K], 1.0133E5[Pa])	J/(mol*K)	Heat capacity (Cp) 2
HeatCapacityCp_hydrogen_Gas15(2000[K],1.0133E5[Pa])	J/(mol*K)	Heat capacity (Cp) 3
HeatCapacityCp_nitrogen_Gas17(2000[K],1.0133E5[Pa])	J/(mol*K)	Heat capacity (Cp) 4
HeatCapacityCp_oxygen_Gas19(2000[K],1.0133E5[Pa])	J/(mol*K)	Heat capacity (Cp) 5
HeatCapacityCp_water_Gas111(2000[K],1.0133E5[Pa])	J/(mol*K)	Heat capacity (Cp) 6

4 In the **Evaluation Group 1** toolbar, click **Evaluate**.

The values in rows 7-12 in the table from **Evaluation Group 1** are for 300 K, while the values for rows 13-18 are for 2000 K. Together with the values in rows 1-6, these are presented in Table 1 and Table 2.

STUDY 1

Solution 1 (sol1)

1 In the **Model Builder** window, under **Study 1>Solver Configurations** right-click **Solution 1 (sol1)** and choose **Compute**.

The default plots that are supposed to be generated when clicking **Compute** were not generated this time because they had already been generated when performing the **Get initial values** step. Therefore, they need to be reset.

2 In the **Study** toolbar, click **Reset Default Plots**.

Now move on to postprocess the result from the nonisothermal jet. Start by creating a **Mirror 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 relevant plot groups.

Velocity (spf)

1 In the **Model Builder** window, under **Results** 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**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1 (comp1)> Heat Transfer in Fluids>Velocity and pressure>ht.ur,ht.uz - Velocity field**.

3 Locate the **Streamline Positioning** section. 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, under **Results** 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, under **Results** 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 correspond 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 22

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

Line Graph 1

1 Right-click **1D Plot Group 22** 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 22** 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 Click to expand the **Legends** section. Select the **Show legends** check box.

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

15 In the table, enter the following settings:

Legends
Exp.

T @ centerline

1 In the **Model Builder** window, under **Results** click **1D Plot Group 22**.

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

3 Locate the **Plot Settings** section.

4 Select the **x-axis label** check box. In the associated text field, type `(z-Pl)/Di`.

5 Select the **y-axis label** check box. In the associated text field, type `T/T0`.

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

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

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

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

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

11 Locate the **Legend** section. From the **Layout** list, choose **Outside graph axis area**.

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 23

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 23** 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 23** toolbar, click **Plot**.

Table Graph 1

1 In the **Model Builder** window, right-click **1D Plot Group 23** 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 Locate 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
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 From the **Positioning** list, choose **Interpolated**.

6 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 23**.

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.

6 Select the **x-axis label** check box. In the associated text field, type `r/Di`.

7 Select the **y-axis label** check box. In the associated text field, type `T/T0`.

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

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

10 In the **x maximum** text field, type `10`.

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

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

13 Locate the **Legend** section. From the **Layout** list, choose **Outside graph axis area**.

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 From the **Title type** list, choose **Manual**.

4 In the **Title** text area, type `Axial Velocity Downstream of the Pipe Exit`.

5 Locate the **Plot Settings** section. In the **y-axis label** text field, type `uz/Ujet`.

6 Locate the **Axis** section. In the **y minimum** text field, type `-0.25`.

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

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

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**.

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 From the **Positioning** list, choose **Interpolated**.

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

Legends
`N2, Exp`

7 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.

3 Locate the **Title** section. From the **Title type** list, choose **Manual**.

4 In the **Title** text area, type `Mass Fraction Along the Centerline`.

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 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.

3 Locate the **Title** section. From the **Title type** list, choose **Manual**.

4 In the **Title** text area, type `Mass Fraction Along the Centerline`.

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**.