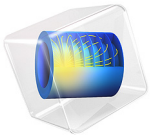

Dissociation in a Tubular Reactor

Introduction

Tubular reactors are often used in continuous large-scale production, for example in the petroleum industry. One key design and optimization parameter is the conversion, or the amount of reactant that reacts to form the desired product. In order to achieve high conversion, process engineers optimize the reactor design: its length, width and heating system. An accurate reactor model is a very useful tool, both at the design stage and in tuning an existing reactor.

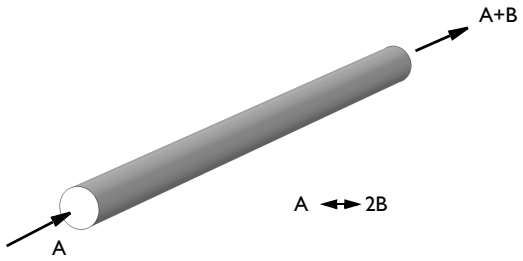

Figure 1: Dissociation reaction in a tubular reactor.

This example deals with a gas-phase dissociation process, species A reacts to form B (see Figure 1). The following physics interfaces are used:

- Chemistry.
- Laminar Flow with compressible formulation.
- Transport of Concentrated Species.
- Heat Transfer in Fluids.

Model Definition

KEY INSTRUCTIVE ELEMENTS

This model illustrates several attractive features in the Chemical Reaction Engineering Module:

- Using Transport of Concentrated Species to account for multicomponent diffusion.
- Implementation of temperature- and composition-dependent reaction kinetics.
- How to use the Reacting Flow multiphysics coupling to account for reaction kinetics in the Single-Phase Flow and Heat Transfer in Fluids interface. Composition dependent

properties, as well as the resulting heat source, are defined automatically by the Chemistry interface.

- Defining user-defined species and including them in a thermodynamic system.
- The use of a mapped mesh to discretize a slender geometry, typical for tubular reactors.

HANDLING THERMAL AND TRANSPORT PROPERTIES — CHEMISTRY

The molecule N_2O_4 is a dimer which exists in a strongly temperature dependent equilibrium:

$$N_2O_4 \leftrightarrow 2NO_2$$

The kinetics of reaction is defined as

$$-R_{N_2O_4} = k_f c_{N_2O_4} - \frac{k_f}{K_{eq}} c_{NO_2}$$

where k_f denotes the forward reaction rate constant (SI unit: s^{-1}), c represents the concentration of species (SI unit: mol/m^3) and K_{eq} is the equilibrium constant (dimensionless).

The Chemistry interface coupled with Thermodynamics can provide all species and mixture thermal and transport properties. These properties can be used directly in other physics interfaces. Species and their properties can be selected from the COMSOL database.

The section Modeling Instructions, explains how to add a new species to this database, because nitrogen dioxide (NO_2) and nitrogen tetroxide (N_2O_4) are not available.

HANDLING EXPANDING FLOW — COMPRESSIBLE FLOW FORMULATION

Each mole of the reactant, A, reacts to form two moles of the product, B:

$$A \leftrightarrow 2B$$

This leads to a volumetric expansion of the gas mixture as the reaction proceeds. The fluid's change in density influences the gas velocity in the reactor, causing an acceleration as the reaction proceeds.

In order to model the flow, use a compressible formulation of the Navier-Stokes equations, defined according to the following equations:

$$\rho(\mathbf{u}\cdot\nabla)\mathbf{u} = \nabla\cdot\left[-p\mathbf{I} + \mu(\nabla\mathbf{u} + (\nabla\mathbf{u})^T) - \frac{2}{3}\mu(\nabla\cdot\mathbf{u})\mathbf{I}\right]$$

$$\nabla \cdot (\rho \mathbf{u}) = 0$$

Here ρ denotes the solution's density (SI unit: kg/m^3), $\mathbf{u}$ is the velocity vector (SI unit: m/s), p gives the pressure (SI unit: Pa), μ represents the solution's viscosity (SI unit: kg/(m·s), or Pa·s), and $\mathbf{I}$ denotes the identity matrix.

The density is varying and depends on the *pressure*, *temperature*, and *composition* according to the ideal gas law. This is the default gas phase model, as defined in the Thermodynamics interface's Gas System node under Thermodynamic Model. It is coupled to other interfaces in the model via the Chemistry interface's Mixture Properties section.

The model applies the Laminar Flow interface, which solves the above equations, describing the momentum balances and the continuity (mass conservation) for fluids with variations in density.

CONVECTION AND DIFFUSION IN MULTICOMPONENT SYSTEMS — TRANSPORT OF CONCENTRATED SPECIES

As the dissociation reaction proceeds, the composition of the mixture changes from pure A at the inlet to a mixture of A and B.

The total mass flux is strongly influenced by the flux of each species. In addition, several molecular interactions occur; A interacts with B and other A molecules, B interacts with A and other B molecules. This implies that the simple Fick's law formulation, with one constant diffusivity for each species is not applicable here. In a concentrated multicomponent mixture you must account for all possible interactions, and the flux is dependent on the fluid's local composition. Simple Fick diffusivity accounts only for the interaction between solvent and solute. In the Transport of Concentrated Species with the Maxwell-Stefan or Mixture-Averaged diffusion equations, multicomponent diffusivities describe the interactions between all components in the system.

Since a change in a gas mixture composition affects the density, the species transport equation needs to be coupled with the flow equations (Laminar Flow, Navier-Stokes in this case).

Now consider a mathematical formulation of this discussion. The mass-balance equation for each species is

$$\frac{\partial}{\partial t}(\rho w_{\mathrm{A}}) + \nabla \cdot \mathbf{n}_{\mathrm{A}} = R_{\mathrm{A}}$$

$$\frac{\partial}{\partial t}(\rho w_{\mathrm{B}}) + \nabla \cdot \mathbf{n}_{\mathrm{B}} = R_{\mathrm{B}}$$

where w_{A} and w_{B} are the mass fractions of each component, $\mathbf{n}_{\mathrm{A}}$ and $\mathbf{n}_{\mathrm{B}}$ are the total fluxes of the species (including both convective and diffusive contributions), and R_{A} and R_{B} are given by the reaction kinetics from Chemistry interface. As mentioned earlier, it is possible to rewrite the mass-balances equations for each species by replacing one of the species' mass balance with a total mass balance. A solution with two species follows following equation:

$$\frac{\partial}{\partial t}(\rho(w_A + w_B)) + \nabla \cdot (\mathbf{n}_A + \mathbf{n}_B) = R_A + R_B$$

Because the system consists only of two species, the sum of w_A and w_B is always unity, and the sum of the reaction terms is zero. The above equation now becomes

$$\frac{\partial}{\partial t}\rho + \nabla \cdot (\mathbf{n}_A + \mathbf{n}_B) = 0$$

which is the total mass-balance equation.

GEOMETRY

The geometry of the tubular reactor is rotationally symmetric, and it is possible to reduce the model from 3D to a 2D axisymmetric problem. This means that you only have to model half of the tube cross section, as illustrated in Figure 2.

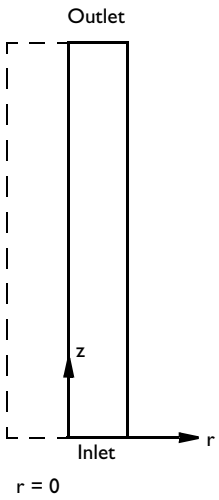

Figure 2: Model geometry.

BOUNDARY CONDITIONS

Laminar Flow interface

The flow in the reactor is driven by Normal inflow velocity at inlet. The walls are represented by no slip boundary conditions $\mathbf{u} = 0$.

Transport of Concentrated Species interface

At the inlet, the mass fraction of A is set close to unity (0.99). The outlet boundary condition is a convective flux condition. The convective flux condition implies that diffusive flux for the species is zero perpendicular to the boundary. This is a common assumption when modeling the outlet in tubular reactors.

No-flux conditions — referred to as insulation/symmetry in COMSOL Multiphysics — apply at all other boundaries. Across these boundaries a no (total) mass flux condition is prescribed for all species.

MESH

In this example, a mapped (structured) mesh is a good choice due to the reactor's regular shape. The use of a structured mesh is especially suitable when the requirements for the mesh density is uneven. In this example a denser mesh is required in the inlet region and

the reactor wall. This is achieved by specifying the edge element distribution, as you see in Modeling Instructions.

Study 1 — Results and Discussion for Isothermal Conditions

Under isothermal conditions, the Laminar Flow and Transport of Concentrated Species interfaces, coupled using a Reacting Flow multiphysics node, are applied to solve the compressible Navier-Stokes equations together with mass transport equations including Maxwell-Stefan diffusion. The Chemistry interface defines the reactions kinetics as well as the transport properties of the fluid mixture. The binary diffusivity and the viscosity are defined dependent on the composition. The Reacting Flow coupling synchronizes the properties and applies them in the coupled interfaces.

Figure 3 shows the velocity magnitude for the isothermal case at different reactor cross sections. The velocity increases along the axis direction (z) because of the volume expansion of gas mixture during the proceeding of reaction.

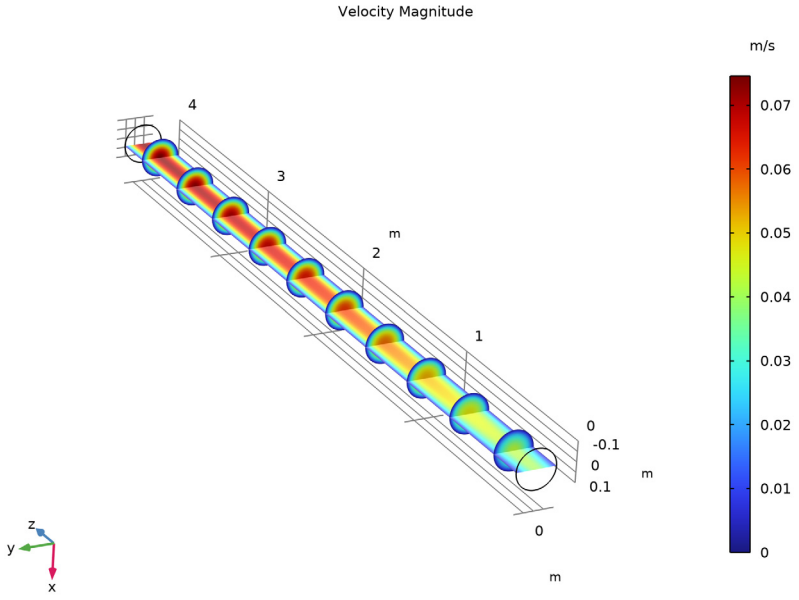

Figure 3: Velocity magnitude for the isothermal case.

Figure 4 shows the mass fraction of species B for the isothermal case at different reactor cross sections. Closer to the reactor walls, the convective flow velocity is lower, due to the

no slip condition on the walls. Consequently the mass fraction of species B increases toward the wall. The average mass fraction of species B at the outlet is 95%.

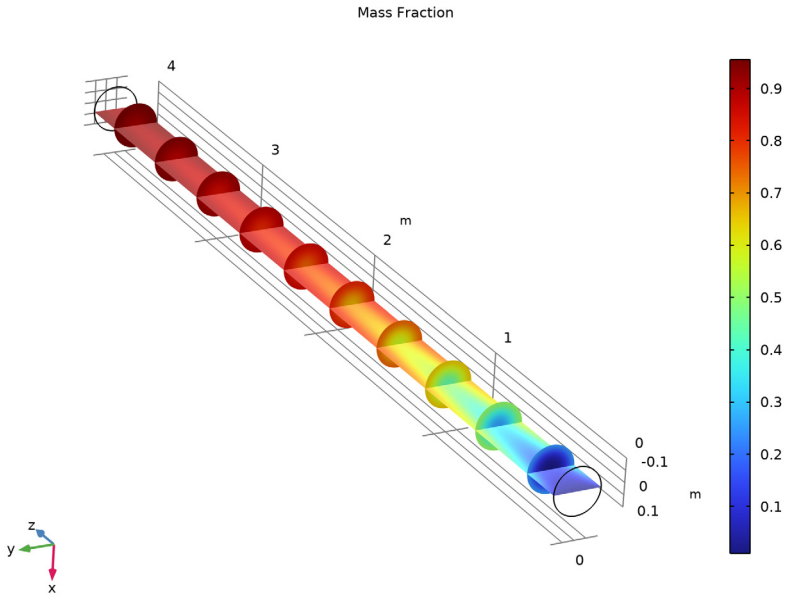

Figure 4: Mass fraction of species B for the isothermal case.

The average conversion rate depends on the flow-rate profile, density distribution, and velocity field. It is defined as

$$\gamma_B = \frac{\int w_B \rho \mathbf{u} \cdot \mathbf{n} ds}{\int \rho \mathbf{u} \cdot \mathbf{n} ds}$$

The average conversion rate at the outlet under isothermal conditions is 94%.

Model Definition — Nonisothermal Model

Now it is time to expand the model by including an energy-balance equation to model a varying temperature field in the reactor. In the previous model, the temperature was constant and set to 500 K. Now assume that the gas enters the reactor at room temperature, 293 K, and that the surroundings outside of the reactor walls is heated to accelerate the reaction. In addition, the heat of reaction is also included, acting as a source term.

The influence of the temperature on the reaction rate is significant. In gas phase, the equilibrium proportion of nitrogen dioxide is greater at higher temperature or lower pressure. Thus, the reaction rate increases as the fluid flows through the reactor and is heated by the walls and by the heat of reaction.

The energy-balance equation is

$$\rho C_p \frac{\partial T}{\partial t} + \nabla \cdot (-k\nabla T) = Q - \rho C_p(\mathbf{u} \cdot \nabla T)$$

where k is the thermal conductivity (SI unit: W/(m·K)), C_p is the specific heat capacity (SI unit: J/(kg·K)), and Q is the heat source term (SI unit: W/m).

The boundary conditions for the energy balance are similar to those of the mass balances. At the inlet, the gas temperature is specified, in this case to 293 K.

The default Axial symmetry condition gives a zero temperature gradient at the symmetry boundary: $\mathbf{n} \cdot \nabla T = 0$. At the outlet, the same equation results in a purely convective flux condition.

Model the reactor's heated walls by applying a heat flux condition on the wall:

$$\mathbf{n} \cdot (k\nabla T) = U(T_f - T)$$

Use the heat transfer coefficient $U = 50$ W/(m^2·K) for the heat transfer to the reactor surroundings, and the heating temperature $T_f = 500$ K.

Study 2 — Results and Discussion for Nonisothermal Conditions

For the nonisothermal case the Heat Transfer in Fluids interface is solved for, along with fluid flow and mass transfer, by coupling it the Reacting Flow node. For a consistent heat transfer a Chemistry interface is required in the coupling. The reason for this is that the Chemistry interface defines the thermodynamic properties of the mixture, the enthalpy and heat capacity, and the excess heat due to the reaction. The properties of each participating species is also needed. In this model this is provided by the user defined species added in Thermodynamics.

Figure 5 shows the velocity magnitude for the nonisothermal case at different cross-sections of reactor. The velocity magnitude for the nonisothermal case is slightly higher than that for the isothermal case (see Figure 3).

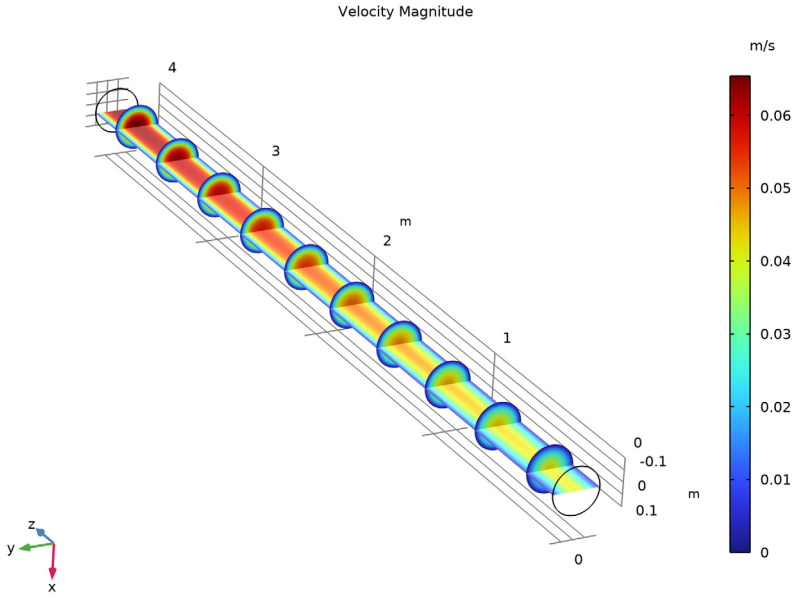

Figure 5: Velocity magnitude for the nonisothermal case.

Figure 6 shows the mass fraction of species B for the nonisothermal case at different cross-sections of reactor. At the region close to the side wall, the mole fraction is much higher than that in the central region due to the higher temperature close to the wall. The overall mole fraction is lower than that for the isothermal conditions (see Figure 4) because of the low temperature in the reactor. The average conversion rate at the outlet is 58% under nonisothermal conditions.

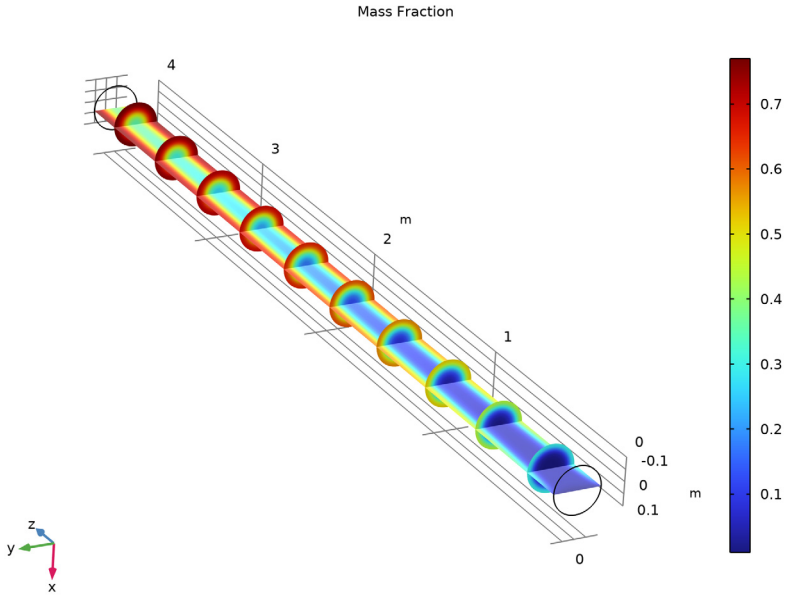

Figure 6: Mass fraction of species B for the nonisothermal case.

Figure 7 shows the temperature distribution under nonisothermal conditions. The temperature is much higher close to the reactor wall. This temperature profile has a significant impact on the reaction rate in the reactor; see Figure 6.

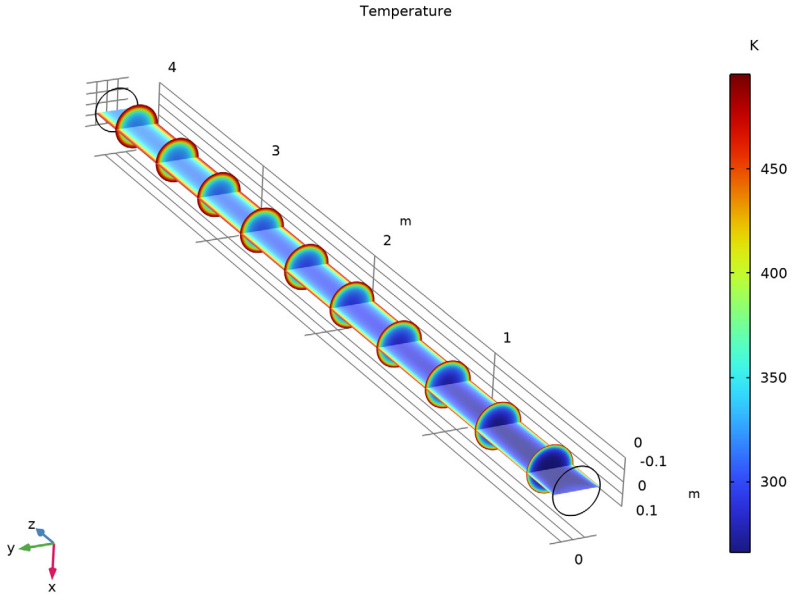

Figure 7: Temperature distribution for nonisothermal case.

Application Library path: `Chemical_Reaction_Engineering_Module/Thermodynamics/dissociation`

Modeling Instructions

From the **File** menu, choose **New**.

NEW

1 In the **New** window, Start by adding the individual physics interfaces for mass transfer, fluid flow, and heat transfer in fluids.

2 click **Model Wizard**.

MODEL WIZARD

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

2 In the **Select Physics** tree, select **Chemical Species Transport>Transport of Concentrated Species (tcs)**.

3 Click **Add**.

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

wA
wB

5 In the **Select Physics** tree, select **Fluid Flow>Single-Phase Flow>Laminar Flow (spf)**.

6 Click **Add**.

7 In the **Select Physics** tree, select **Heat Transfer>Heat Transfer in Fluids (ht)**.

8 Click **Add**.

9 Click **Study**.

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

11 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 `dissociation_parameters.txt`.

Gas System 1 (pp1)

In this model, a **Thermodynamic System** containing **NO2** and **N2O4** is used. Import the pre-defined system from a file. See the Appendix below for details on how to create the system.

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

2 Browse to the model's Application Libraries folder and double-click the file `dissociation_thermo_system.xml`.

Since **NO2** and **N2O4** are not available in the built-in thermodynamics database, they have been created as **User-Defined Species** in the imported file.

GEOMETRY 1

The model geometry is simply a rectangle.

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 `W0`.

4 In the **Height** text field, type `L0`.

5 Click **Build All Objects**.

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

DEFINITIONS

Average 1 (aveop1)

1 In the **Definitions** toolbar, click **Nonlocal Couplings** and choose **Average**.

You will use this function later in the results analysis. With the check box **Compute integral in revolved geometry** enabled, it automatically performs a surface integration by multiplication with 2*pi*r.

2 In the **Settings** window for **Average**, locate the **Source Selection** section.

3 From the **Geometric entity level** list, choose **Boundary**.

4 Select Boundary 3 only.

GLOBAL DEFINITIONS

Use the **Gas System 1** to generate a corresponding **Chemistry** interface.

Gas System 1 (pp1)

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

SELECT SPECIES

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

2 Click **Add All**.

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

CHEMISTRY SETTINGS

1 Go to the **Chemistry Settings** window.

2 From the **Mass transfer** list, choose **Concentrated species**.

3 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 `N2O4<=>NO2`.

4 Click **Apply**.

Now, the reaction is unbalanced. To make it stoichiometrically balanced, click **Balance**.

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

6 Locate the **Rate Constants** section. Select the **Specify equilibrium constant** check box.

7 In the k^{f} text field, type `kf`.

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

9 In the **Settings** window for **Chemistry**, locate the **Species Matching** section.

10 From the **Species solved for** list, choose **Transport of Concentrated Species**.

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

Species	Type	Mass fraction	Value (1)	From Thermodynamics
N2O4	Variable	wA	Solved for	N2O4
NO2	Variable	wB	Solved for	NO2

12 Click to expand the **Calculate Transport Properties** section. Drag and drop below **Materials**.

Now add the **Reacting Flow** multiphysics coupling node. When using the **Chemistry** interface it supports both isothermal and nonisothermal flow.

MULTIPHYSICS

Reacting Flow 1 (nirf1)

In the **Physics** toolbar, click  **Multiphysics Couplings** and choose **Domain>Reacting Flow**.

LAMINAR FLOW (SPF)

Since the density variation is large, the flow cannot be regarded as incompressible. Therefore select **Compressible flow**.

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Laminar Flow (spf)**.

2 In the **Settings** window for **Laminar Flow**, locate the **Physical Model** section.

3 From the **Compressibility** list, choose **Compressible flow (Ma<0.3)**.

Define the pressure reference level in the interface properties.

4 In the p_{ref} text field, type `p_amb`.

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 `v_in`.

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 **Maxwell-Stefan**.

4 Locate the **Species** section. From the **From mass constraint** list, choose **wB**.

Species Molar Masses 1

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

2 In the **Settings** window for **Species Molar Masses**, locate the **Molar Mass** section.

3 From the M_{wA} list, choose **Molar mass (chem/N2O4)**.

4 From the M_{wB} list, choose **Molar mass (chem/NO2)**.

Transport Properties 1

1 In the **Model Builder** window, click **Transport Properties 1**.

2 In the **Settings** window for **Transport Properties**, locate the **Diffusion** section.

3 In the table, enter the following settings:

Species 1	Species 2	Diffusivity	Diffusion coefficient (m^2/s)
wA	wB	Maxwell-Stefan diffusivity , N2O4-NO2 (chem)	comp1.chem.D_N2O4_NO2

Reaction Sources 1

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

2 Select Domain 1 only.

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

4 From the R_{wA} list, choose **Reaction rate for species N2O4 (chem)**.

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 In the $\omega_{0,wA}$ text field, type `wN2O4_in`.

Outflow 1

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

2 Select Boundary 3 only.

MESH 1

A mapped mesh is suitable for fluid flow.

Mapped 1

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

Distribution 1

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

2 Select Boundaries 1 and 4 only.

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

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

5 In the **Number of elements** text field, type `100`.

6 In the **Element ratio** text field, type `50`.

Distribution 2

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

2 Select Boundaries 2 and 3 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 `10`.

6 In the **Element ratio** text field, type `5`.

For the isothermal case decouple the **Heat Transfer in Fluids** interface in the **Reacting Flow** coupling feature. Also apply a constant value `Tf` for the temperature. This is needed to provide the reaction rate and density with a valid temperature.

MULTIPHYSICS

Reacting Flow 1 (nirf1)

1 In the **Model Builder** window, under **Component 1 (comp1)>Multiphysics** click **Reacting Flow 1 (nirf1)**.

2 In the **Settings** window for **Reacting Flow**, locate the **Coupled Interfaces** section.

3 From the **Heat transfer (optional, requires Chemistry)** list, choose **None**.

4 Locate the **Temperature** section. In the T text field, type `Tf`.

STUDY - ISOTHERMAL MODEL

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

2 In the **Settings** window for **Study**, type `Study - Isothermal Model` in the **Label** text field.

3 Locate the **Study Settings** section. Clear the **Generate default plots** check box.

Step 1: Stationary

Turn off the **Heat Transfer in Fluids** interface to avoid solving for the temperature.

1 In the **Model Builder** window, under **Study - Isothermal Model** click **Step 1: Stationary**.

2 In the **Settings** window for **Stationary**, locate the **Physics and Variables Selection** section.

3 In the table, clear the **Solve for** check box for **Heat Transfer in Fluids (ht)**.

4 In the **Home** toolbar, click **Compute**.

RESULTS

Global Evaluation 1

1 In the **Model Builder** window, expand the **Results** node.

2 Right-click **Results>Derived Values** and choose **Global Evaluation**.

3 In the **Settings** window for **Global Evaluation**, locate the **Expressions** section.

4 In the table, enter the following settings:

Expression	Unit	Description
`aveop1(w*spf.rho*wB)/aveop1(w*spf.rho)`	1	

5 Click ▼ next to **Evaluate**, then choose **New Table**.

Revolution 2D 1

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

Velocity, isothermal

1 In the **Results** toolbar, click **3D Plot Group**.

2 In the **Settings** window for **3D Plot Group**, type `Velocity, isothermal` in the **Label** text field.

Slice 1

1 Right-click **Velocity, isothermal** and choose **Slice**.

2 In the **Settings** window for **Slice**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1 (comp1)>Laminar Flow> Velocity and pressure>spf.U - Velocity magnitude - m/s**.

3 Locate the **Plane Data** section. From the **Plane** list, choose **xy-planes**.

4 In the **Planes** text field, type `10`.

5 Locate the **Coloring and Style** section. Clear the **Color legend** check box.

Slice 2

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

2 In the **Settings** window for **Slice**, locate the **Plane Data** section.

3 From the **Plane** list, choose **yz-planes**.

4 In the **Planes** text field, type `1`.

5 Locate the **Coloring and Style** section. Select the **Color legend** check box.

6 Click to expand the **Title** section. From the **Title type** list, choose **None**.

7 In the **Velocity, isothermal** toolbar, click **Plot**.

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

Mass fraction, B, isothermal

1 In the **Model Builder** window, right-click **Velocity, isothermal** and choose **Duplicate**.

2 In the **Settings** window for **3D Plot Group**, type `Mass fraction, B, isothermal` in the **Label** text field.

Slice 1

1 In the **Model Builder** window, expand the **Mass fraction, B, isothermal** node, then click **Slice 1**.

2 In the **Settings** window for **Slice**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1 (comp1)>Transport of Concentrated Species>Species wB>wB - Mass fraction**.

Slice 2

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

2 In the **Settings** window for **Slice**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1 (comp1)>Transport of Concentrated Species>Species wB>wB - Mass fraction**.

3 In the **Mass fraction, B, isothermal** toolbar, click **Plot**.

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

Add a new study for the nonisothermal simulation. This makes it straightforward to compare results from the two setups.

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.

STUDY - NONISOTHERMAL MODEL

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

2 In the **Settings** window for **Study**, type `Study - Nonisothermal Model` in the **Label** text field.

Now set up the **Heat Transfer in Fluids** interface. Note that the heat source due to reactions is automatically accounted for when **Chemistry** is included in the **Reacting Flow** coupling feature. Hence there is no need to add a **Heat Source** feature in **Heat Transfer in Fluids**.

HEAT TRANSFER IN FLUIDS (HT)

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

Outflow 1

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

2 Select Boundary 3 only.

Temperature 1

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

2 Select Boundary 2 only.

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

4 In the T_0 text field, type `T_amb`.

Heat Flux 1

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

2 Select Boundary 4 only.

3 In the **Settings** window for **Heat Flux**, locate the **Heat Flux** section.

4 In the q_0 text field, type `Ua*(Tf-T)`.

For the nonisothermal case reenable the **Heat Transfer in Fluids** interface in the **Reacting Flow** coupling feature. This synchronizes the temperature solved for among all other coupled interfaces. The thermodynamic properties of the mixture are defined by the **Chemistry** interface.

MULTIPHYSICS

Reacting Flow 1 (nirf1)

1 In the **Model Builder** window, under **Component 1 (comp1)>Multiphysics** click **Reacting Flow 1 (nirf1)**.

2 In the **Settings** window for **Reacting Flow**, locate the **Coupled Interfaces** section.

3 From the **Heat transfer (optional, requires Chemistry)** list, choose **Heat Transfer in Fluids (ht)**.

STUDY - NONISOTHERMAL MODEL

1 In the **Model Builder** window, click **Study - Nonisothermal Model**.

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

3 Clear the **Generate default plots** check box.

4 In the **Home** toolbar, click **Compute**.

RESULTS

Global Evaluation 2

1 In the **Model Builder** window, under **Results>Derived Values** right-click **Global Evaluation 1** and choose **Duplicate**.

2 In the **Settings** window for **Global Evaluation**, locate the **Data** section.

3 From the **Dataset** list, choose **Study - Nonisothermal Model/Solution 2 (sol2)**.

4 Click ▼ next to **Evaluate**, then choose **Table 1 - Global Evaluation 1**.

Revolution 2D 2

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

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

3 From the **Dataset** list, choose **Study - Nonisothermal Model/Solution 2 (sol2)**.

Velocity, nonisothermal

1 In the **Model Builder** window, right-click **Velocity, isothermal** and choose **Duplicate**.

2 In the **Settings** window for **3D Plot Group**, type `Velocity, nonisothermal` in the **Label** text field.

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

4 Locate the **Plot Settings** section. From the **View** list, choose **View 3D 2**.

Slice 1

1 In the **Model Builder** window, expand the **Velocity, nonisothermal** node, then click **Slice 1**.

2 In the **Velocity, nonisothermal** toolbar, click **Plot**.

3 In the **Settings** window for **Slice**, in the **Graphics** window toolbar, click ▼ next to **Go to Default View**, then choose **Go to View 3D 2**.

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

Mass fraction B, nonisothermal

1 In the **Model Builder** window, right-click **Mass fraction, B, isothermal** and choose **Duplicate**.

2 In the **Settings** window for **3D Plot Group**, type `Mass fraction B, nonisothermal` in the **Label** text field.

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

4 In the **Mass fraction B, nonisothermal** toolbar, click **Plot**.

5 Locate the **Plot Settings** section. From the **View** list, choose **View 3D 2**.

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

Temperature

1 Right-click **Mass fraction B, nonisothermal** and choose **Duplicate**.

2 In the **Settings** window for **3D Plot Group**, type `Temperature` in the **Label** text field.

3 In the **Temperature** toolbar, click **Plot**.

Slice 1

1 In the **Model Builder** window, expand the **Temperature** node, then click **Slice 1**.

2 In the **Settings** window for **Slice**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1 (comp1)>Heat Transfer in Fluids>Temperature>T - Temperature - K**.

Slice 2

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

2 In the **Settings** window for **Slice**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1 (comp1)>Heat Transfer in Fluids>Temperature>T - Temperature - K**.

3 In the **Temperature** toolbar, click **Plot**.

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

Appendix

Follow the steps below to create the thermodynamic system used in the model. Two **User-Defined Species** are also created.

From the **File** menu, choose **New**.

NEW

In the **New** window, click **Blank Model**.

GLOBAL DEFINITIONS

In the **Physics** toolbar, click **Thermodynamics** and choose **User-Defined Species**.

ENTER NAME AND FORMULA

1. Go to the **Enter Name and Formula** window.
2. In the text field, type `N2O4`.
3. In the text field, type `10544-72-6`.
4. In the text field, type `N2O4`.
5. Click **Next** in the window toolbar.

ENTER PARAMETERS

1. Go to the **Enter Parameters** window.
2. Find the **Constants** subsection. In the table, enter the following settings:

Name	Values	Unit
Absolute entropy	304.32	J/mol/K
Critical compressibility factor	0.233	1
Critical pressure	1.0031e+07	Pa
Critical temperature	431.15	K
Critical volume	8.249e-05	m^3/mol
Molecular mass	92.011	g/mol
Normal boiling point temperature	294.3	K
Standard enthalpy of formation	9163	J/mol
van der Waals area	0	m^2/mol
van der Waals volume	0	m^3/mol

3 Find the **Model parameters** subsection. In the table, enter the following settings:

Name	Values	Unit
Acentric factor	0.85327	1

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

DEFINE PROPERTIES

1 Go to the **Define Properties** window.

2 Find the **Heat capacity (J/(K*mol))** subsection. Click + **Add**.

3 In the **Ideal gas** table, enter the following settings:

T(K), low	a0	a1	a2	a3	T(K), high
151.4994	22.8199439173	0.248101835092	-0.000129016784375	-2.07976512868e-07	223.9986

4 Click + **Add**.

5 In the **Ideal gas** table, enter the following settings:

T(K), low	a0	a1	a2	a3	T(K), high
223.9986	17.3772455746	0.320995572054	-0.000454437286832	2.7628321384e-07	310.9977

6 Click + **Add**.

7 In the **Ideal gas** table, enter the following settings:

T(K), low	a0	a1	a2	a3	T(K), high
310.9977	7.55672923384	0.415727941528	-0.000759045229188	6.02767881686e-07	325.4976

8 Click + **Add**.

9 In the **Ideal gas** table, enter the following settings:

T(K), low	a0	a1	a2	a3	T(K), high
325.4976	23.1617866623	0.271901466969	-0.000317178762095	1.50264322937e-07	557.4951

10 Click + **Add**.

11 In the **Ideal gas** table, enter the following settings:

T(K), low	a0	a1	a2	a3	T(K), high
557.4951	41.6009681157	0.172676299817	-0.000139194835147	4.38454940552e-08	803.9924

12 Click + **Add**.

13 In the **Ideal gas** table, enter the following settings:

T(K), low	a0	a1	a2	a3	T(K), high
803.9924	59.0032311688	0.107741868801	-5.84298540152e-05	1.036052532e-08	1499.985

14 Find the **Saturated liquid density (mol/m^3)** subsection. In the **Natural logarithm liquid viscosity** table, enter the following settings:

T(K), low	a0	a1	a2	a3	T(K), high
261.9	23723.3913174	-54.5872209623	0.161934291432	-0.000237308754858	343.1466

15 Find the **Thermal conductivity (W/(K*m))** subsection. Click + **Add**.

16 In the **Vapor** table, enter the following settings:

T(K), low	a0	a1	a2	a3	T(K), high
380.0038	29.7807267369	-0.219234326434	0.000540095868453	-4.44593410339e-07	400

17 Find the **Vapor viscosity (Pa*s)** subsection. Click + **Add**.

18 In the **Vapor viscosity** table, enter the following settings:

T(K), low	a0	a1	a2	a3	T(K), high
300.003	1.631159576 29e-05	- 1.409301058 36e-07	6.483836631 56e-10	- 6.820538383 04e-13	335.002 35

19 Click + **Add**.

20 In the **Vapor viscosity** table, enter the following settings:

T(K), low	a0	a1	a2	a3	T(K), high
335.002 35	- 9.55153890 719e-06	9.06784306 719e-08	- 4.29802526 723e-11	5.86563034 883e-15	558.69014 735

21 Click + **Add**.

22 In the **Vapor viscosity** table, enter the following settings:

T(K), low	a0	a1	a2	a3	T(K), high
558.69014 735	- 1.14075878 119e-05	1.00644861 511e-07	- 6.08191762 446e-11	1.65089321 605e-14	999.99

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

Define species **NO2**.

GLOBAL DEFINITIONS

In the **Physics** toolbar, click **Thermodynamics** and choose **User-Defined Species**.

ENTER NAME AND FORMULA

1 Go to the **Enter Name and Formula** window.

2 In the text field, type NO2.

3 In the text field, type 10102-44-0.

4 In the text field, type NO2.

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

ENTER PARAMETERS

1 Go to the **Enter Parameters** window.

2 Find the **Constants** subsection. In the table, enter the following settings:

Name	Values	Unit
Absolute entropy	239.92	J/mol/K
Critical compressibility factor	0.233	1
Critical pressure	10132500	Pa
Critical temperature	431.15	K
Critical volume	8.249e-05	m^3/mol
Molecular mass	46.0055	g/mol
Normal boiling point temperature	294.15	K
Standard enthalpy of formation	33180	J/mol

3 Find the **Model parameters** subsection. In the table, enter the following settings:

Name	Values	Unit
Acentric factor	0.851088	1

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

DEFINE PROPERTIES

1 Go to the **Define Properties** window.

2 Find the **Heat capacity (J/(K*mol))** subsection. Click **Add**.

3 In the **Ideal gas** table, enter the following settings:

T(K), low	a0	a1	a2	a3	T(K), high
165.9993	35.8254425805	-0.0567293232053	0.000356001767705	-4.7800454454 1e-07	223.9986

4 Click **Add**.

5 In the **Ideal gas** table, enter the following settings:

T(K), low	a0	a1	a2	a3	T(K), high
223.9986	32.4036320949	-0.0109012177757	0.000151410 73262	-1.7355169665 7e-07	310.9977

6 Click **Add**.

7 In the **Ideal gas** table, enter the following settings:

T(K), low	a0	a1	a2	a3	T(K), high
310.9977	27.9650785955	0.0319147274807	1.37378647707e-05	-2.59912614739e-08	470.49

8 Click + **Add**.

9 In the **Ideal gas** table, enter the following settings:

T(K), low	a0	a1	a2	a3	T(K), high
470.49	24.2998355133	0.055285232749	-3.5934194648e-05	9.20001143717e-09	963.4907

10 Find the **Saturated liquid density (mol/m^3)** subsection. In the **Natural logarithm liquid viscosity** table, enter the following settings:

T(K), low	a0	a1	a2	a3	T(K), high
261.9026	47780.8048854	-96.0025964011	0.26232127372	-0.000423346367284	327.9932

11 Click + **Add**.

12 In the **Natural logarithm liquid viscosity** table, enter the following settings:

T(K), low	a0	a1	a2	a3	T(K), high
327.9932	103808.217268	-608.459065462	1.82472094865	-0.00201118383356	373.7483

13 Click + **Add**.

14 In the **Natural logarithm liquid viscosity** table, enter the following settings:

T(K), low	a0	a1	a2	a3	T(K), high
373.7483	350445.755442	-2588.167373322	7.121623457	-0.006735310122 43	392.3892

15 Click + **Add**.

16 In the **Natural logarithm liquid viscosity** table, enter the following settings:

T(K), low	a0	a1	a2	a3	T(K), high
392.3892	1568690.00637	-11902.2176906	30.8583886824	-0.0268996140205	407.6409

17 Click + **Add**.

18 In the **Natural logarithm liquid viscosity** table, enter the following settings:

T(K), low	a0	a1	a2	a3	T(K), high
407.6409	2741379.02684	-20532.5270178	52.0297415255	-0.0442117081071	414.4194

19 Click + **Add**.

20 In the **Natural logarithm liquid viscosity** table, enter the following settings:

T(K), low	a0	a1	a2	a3	T(K), high
414.4194	23901405.4952	-173710.875824	421.651310414	-0.341512436861	421.1979

21 Click + **Add**.

22 In the **Natural logarithm liquid viscosity** table, enter the following settings:

T(K), low	a0	a1	a2	a3	T(K), high
421.1979	-24025981.4299	167653.980875	-388.81060475	0.299881956897	424.5872

23 Click + **Add**.

24 In the **Natural logarithm liquid viscosity** table, enter the following settings:

T(K), low	a0	a1	a2	a3	T(K), high
424.5872	1171039730.24	-8276305.55206	19498.6460424	-15.3132882369	426.2818

25 Click + **Add**.

26 In the **Natural logarithm liquid viscosity** table, enter the following settings:

T(K), low	a0	a1	a2	a3	T(K), high
426.2818	-3800925140.26	26714385.1401	-62584.8271252	48.872322602	427.9764

27 Click + **Add**.

28 In the **Natural logarithm liquid viscosity** table, enter the following settings:

T(K), low	a0	a1	a2	a3	T(K), high
427.9764	17346687004.3	-121524715.039	283787.3097	-220.90278402	429.6711

29 Click + **Add**.

30 In the **Natural logarithm liquid viscosity** table, enter the following settings:

T(K), low	a0	a1	a2	a3	T(K), high
429.6711	-22629305820.2	157591051.588	-365815.995308	283.051135623	431.3657

31 Find the **Thermal conductivity (W/(K*m))** subsection. Click + **Add**.

32 In the **Vapor** table, enter the following settings:

T(K), low	a0	a1	a2	a3	T(K), high
420.0042	-15.8305048878	0.11194015 1375	-0.000264111354853	2.08523312366e-07	425.804058

33 Click + **Add**.

34 In the **Vapor** table, enter the following settings:

T(K), low	a0	a1	a2	a3	T(K), high
425.804058	0.142692610769	-0.000598918170081	1.86430549483e-07	1.62236779811e-09	483.75782068

35 Click + **Add**.

36 In the **Vapor** table, enter the following settings:

T(K), low	a0	a1	a2	a3	T(K), high
483.75782068	0.568403779574	-0.00323894475326	5.64376161541e-06	-2.13800625176e-09	530.260979312

37 Click + **Add**.

38 In the **Vapor** table, enter the following settings:

T(K), low	a0	a1	a2	a3	T(K), high
530.260979312	4.28090087709	-0.0242427367105	4.52540531072e-05	-2.70378782249e-08	605.722503968

39 Click + **Add**.

40 In the **Vapor** table, enter the following settings:

T(K), low	a0	a1	a2	a3	T(K), high
605.722503968	3.542805559853	-0.0205871257316	3.92189281862e-05	-2.37167067416e-08	651.762146706

41 Click + **Add**.

42 In the **Vapor** table, enter the following settings:

T(K), low	a0	a1	a2	a3	T(K), high
651.762146706	-8.521922611186	0.034945686068	-4.598517819874e-05	1.98595721224e-08	744.873800587

43 Click + **Add**.

44 In the **Vapor** table, enter the following settings:

T(K), low	a0	a1	a2	a3	T(K), high
744.87380587	-6.691047805 57	0.0275717867906	-3.608565074 61e-05	1.542950259 77e-08	791.067898284

45 Find the **Vapor viscosity (Pa*s)** subsection. Click **Add**.

46 In the **Vapor viscosity** table, enter the following settings:

T(K), low	a0	a1	a2	a3	T(K), high
300.003	0.000239189260846	-2.409144420 54e-06	8.253321071 35e-09	-9.099492928 19e-12	307.0029

47 Click **Add**.

48 In the **Vapor viscosity** table, enter the following settings:

T(K), low	a0	a1	a2	a3	T(K), high
307.0029	-1.898101390 51e-05	1.136683094 12e-07	3.576765425 72e-11	-1.771522194 67e-13	335.0023

49 Click **Add**.

50 In the **Vapor viscosity** table, enter the following settings:

T(K), low	a0	a1	a2	a3	T(K), high
335.0023	-3.285009332 25e-05	2.378681678 97e-07	-3.349756465 66e-10	1.917440546 02e-13	488.9995

51 Click **Add**.

52 In the **Vapor viscosity** table, enter the following settings:

T(K), low	a0	a1	a2	a3	T(K), high
488.9995	-2.442117017 96e-05	1.861569300 97e-07	-2.292265858 81e-10	1.196587316 21e-13	579.9978

53 Click **Add**.

54 In the **Vapor viscosity** table, enter the following settings:

T(K), low	a0	a1	a2	a3	T(K), high
579.9978	-1.03829719748e-05	1.13545284649e-07	-1.04033618859e-10	4.77084776588e-14	684.9958

55 Click + **Add**.

56 In the **Vapor viscosity** table, enter the following settings:

T(K), low	a0	a1	a2	a3	T(K), high
684.9958	1.95668473445e-06	5.95026611349e-08	-2.51387942283e-11	9.31660010734e-15	999.99

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

Create a **Thermodynamic System** including the created species.

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

3 Click **Add All**.

4 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)

1. In the **Model Builder** window, under **Global Definitions>Thermodynamics** right-click **Gas System 1 (pp1)** and choose **Export Thermodynamic System**.
2. Browse to a suitable folder, enter the filename `dissociation_thermo_system.xml`, and then click **Save**.