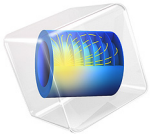


Analysis of NOx Reaction Kinetics

Introduction

This example looks at the reduction of NO by ammonia. The reaction is critical to purify vehicle exhaust gases from NO. In these cases, the reaction usually takes place within the channels of a monolithic reactor situated within the exhaust system.

Central for the monolithic reactor is that NH_3 is present in amounts that do not limit the NO reduction reaction. At the same time, excess NH_3 at the outlet of the reactor leads to undesirable waste. The situation is complicated by the fact that ammonia can be depleted by oxidation, a reaction that is parallel to the NO reduction, and that the rates of the two competing reactions are affected by temperature as well as composition.

This tutorial aims at getting a primary understanding of the monolithic reactor. It concentrates on the investigation of the selectivity of the reactions by solving the model with the Plug Flow ideal reactor type in the Reaction Engineering interface.

Model Definition

CHEMICAL REACTIONS

NO reduction by ammonia can be summarized by the following reaction:

(1)

$$4NO + 4NH_3 + O_2 \longrightarrow 4N_2 + 6H_2O$$

However, ammonia can at the same time undergo oxidation:

(2)

$$4NH_3 + 3O_2 \longrightarrow 2N_2 + 6H_2O$$

The heterogeneous catalytic conversion of NO to N_2 is described by an Eley-Rideal mechanism. A key reaction step involves the reaction of gas-phase NO with surface-adsorbed NH_3. The following rate equation (SI unit: mol/(m^3·s)) has been suggested in Ref. 1 for Equation 1:

$$r_1 = k_1 c_{NO} \frac{a c_{NH3}}{1 + a c_{NH3}}$$

where

$$k_1 = A_1 \exp\left(-\frac{E_1}{R_g T}\right)$$

and

$$a = a_0 \exp\left(-\frac{E_0}{R_g T}\right)$$

For Equation 2, the reaction rate (SI unit: mol/(m^3·s)) is given by

$$r_2 = k_2 c_{NH3} \tag{3}$$

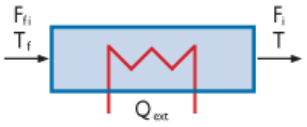
where

$$k_2 = A_2 \exp\left(-\frac{E_2}{R_g T}\right)$$

The competing chemical reactions raise the issue of optimal dosing of NH_3 to handle the reduction process. Stoichiometry suggests a 1:1 ratio of NH_3 to NO as a lower limit. It is likely that a stoichiometric excess of NH_3 is necessary but, at the same time, we want to avoid unnecessarily high levels of NH_3 in the gas stream leaving the catalytic converter.

SINGLE CHANNEL MODEL

To find the minimal level of NH_3 required to reduce the NO present in the exhaust gas requires a reactor model accounting for changing reactant compositions and system temperature. From a mass transfer point of view, channels of the reactor monolith can be considered to be uncoupled to one another. Therefore, it is reasonable to perform simulations where a single reactive channel, modeled by nonisothermal plug flow equations, represents the monolith reactor. These equations are available within the Plug-flow reactor type in the Reaction Engineering interface.



MODEL EQUATIONS

Assuming steady state, the mass balance equation for a plug-flow reactor is:

$$\frac{dF_i}{dV} = R_i \tag{4}$$

where F_i is the species molar flow rate (SI unit: mol/s), V represents the reactor volume (SI unit: m^3), and R_i is the species net reaction rate (SI unit: mol/(m^3·s)). The molar flow rate is related to the species concentrations, c_i (SI unit: mol/m^3), through the volumetric flow rate, v (SI unit: m^3/s):

$$F_i = vc_i \tag{5}$$

where the volumetric flow rate is given by the average flow velocity, u (SI unit: m/s), multiplied by the reactor cross-section A (SI unit: m^2):

$$v = uA \tag{6}$$

The energy balance for the ideal reacting gas is:

$$\sum_i F_i C_{p,i} \frac{dT}{dV} = Q_{\text{ext}} + Q \tag{7}$$

where $C_{p,i}$ is the species molar heat capacity (SI unit: J/(mol·K)), and Q_{ext} is the heat added to the system per unit volume (SI unit: J/(m^3·s)). Q denotes the heat due to chemical reaction (SI unit: J/(m^3·s))

$$Q = -\sum_j H_j r_j$$

where H_j is the heat of reaction (SI unit: J/mol) for reaction j, and r_j the reaction rate (SI unit: mol/(m^3·s)).

The model is first solved with Equation 4, Equation 5, and Equation 6 for several different ratios of reactant concentrations (NH_3:NO) and with a temperature ramp along the reactor. The molar flow rates of NH_3 and NO are kept constant throughout the reactor to investigate the temperature impact alone. Thereafter, Equation 7 is included; that is, nonisothermal conditions due to heat of reaction are studied.

Results and Discussion

REACTION KINETICS ANALYSIS

Analyzing the kinetics can help narrow down a proper NH_3:NO ratio. A first study looks at the reaction rates of the reduction and oxidation reactions, for fixed molar flow rates of

NH_3 and NO, as function of temperature and relative amounts of reactants. Figure 1 shows the reaction rates for the reduction reaction (reaction 1 above). The curves represent a set of NH_3:NO ratios (*X0*) ranging from 1 to 2. The concentration of NO in the exhaust gas entering the catalytic converter is known to be 0.0411 mol/m^3.

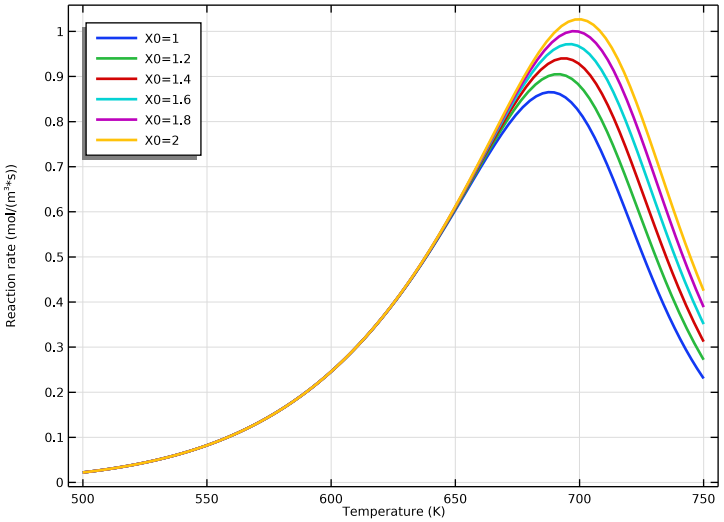


Figure 1: Reaction rates of the NO reduction reaction (r_1) as a function of temperature. The NH_3:NO ratio ranges from 1 to 2 and the molar flow rates of NH_3 and NO are kept constant throughout the reactor.

The rate of NO reduction goes through a maximum and falls off at higher temperatures. The maximum shifts toward higher temperatures as the ratio NH_3:NO increases. This behavior is explained by the desorption rate of NH_3 from the catalyst surface becoming faster than the reaction of adsorbed NH_3 with gas-phase NO.

According to Equation 3, the oxidation rate increases with increased temperature and NH_3 concentration. This is seen in Figure 2, plotting the selectivity parameter S as a function of reactant ratio and temperature. S is defined as the ratio of reaction rates:

$$S = \frac{r_1}{r_2}.$$

An S-value greater than one means that NO reduction is favored.

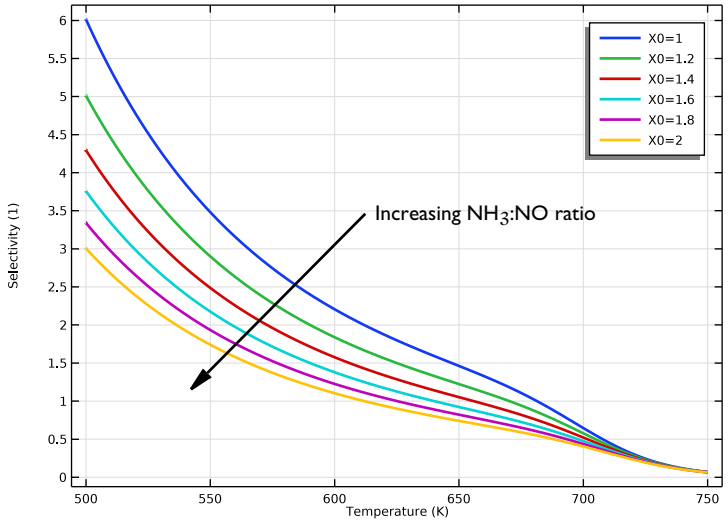


Figure 2: Selectivity parameter (r_1/r_2) as a function of temperature. The NH_3:NO ratio ranges from 1 to 2.

The kinetic analysis suggests that preferred working conditions involve moderate temperatures and relatively low ratios of NH_3:NO.

SINGLE CHANNEL MODEL

To find the minimal level of NH_3 required to reduce the NO present in the exhaust gas requires a reactor model accounting for changing reactant concentrations and system temperature. For this purpose, a nonisothermal plug-flow reactor serves to simulate the behavior of a reactive channel.

For an exhaust gas containing 41.1 mmol/m^3 of NO, with a temperature of 523 K, passing through the monolith at 0.3 m/s, the plug-flow model suggests a NH_3:NO ratio higher than 1.2 to guarantee that NH_3 is available as a reductive agent throughout the

entire length of the reactive channel, see Figure 3. The reactor is 0.36 m long and has a volume of 45e-5 m^3.

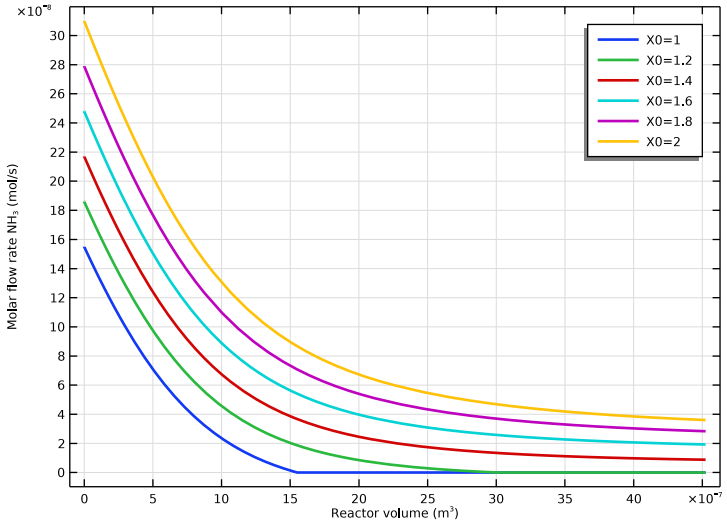


Figure 3: Molar flow rate of NH_3 as function of channel volume.

A plot of the selectivity parameter (Figure 4) confirms that the NO reduction chemistry is favored in the monolith reactor at NH_3:NO ratios ranging from 1.3 to 1.5.

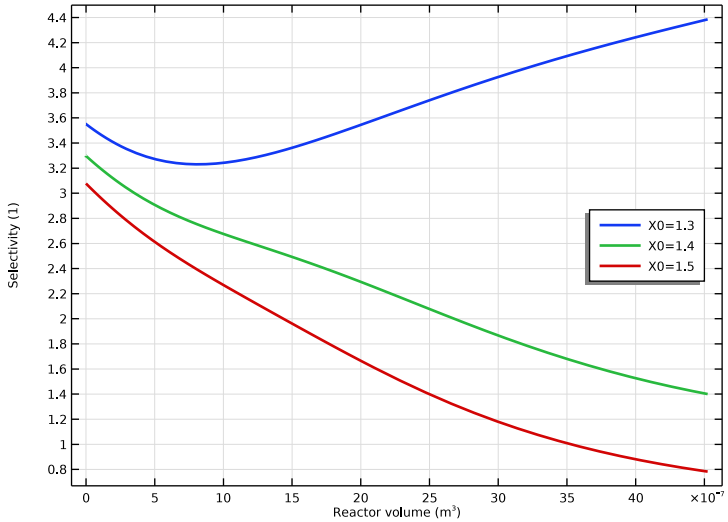


Figure 4: Selectivity parameter (r_1/r_2) as a function of channel volume. The NH_3:NO ratio ranges from 1.3 to 1.5.

Finally, Figure 5 shows the temperature, as well as the conversion of NO, throughout the single channel reactor. The maximum values for these properties are included. The highest temperature in the reactor is 532K for $X0$ = 1.3, and 533 K for $X0$ = 1.5. The conversion of NO is practically 1 (99%) for both $X0$ values.

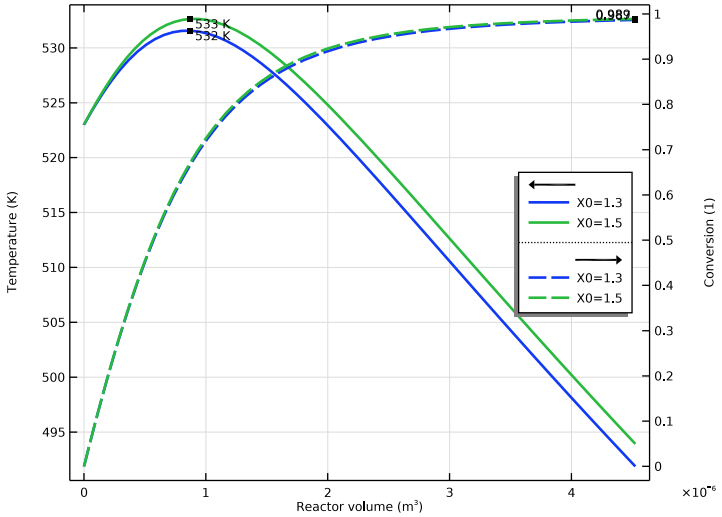


Figure 5: Temperature and conversion as a function of channel volume.

It is clear that temperature plays a central role in affecting the optimal dosing of NH_3. Since the temperature distribution is likely to vary from channel to channel in a monolith reactor, a full 3D reactor model is called for. Based on the single channel model simulations, a NH_3:NO ratio between 1.3 and 1.4 appears appropriate for the 3D model.

Note: For details on the full 3D model of the reactor monolith, see the example `monolith_3d.mph` in the Chemical Reaction Engineering Module's Application Libraries.

Application Library path: `Chemical_Reaction_Engineering_Module/Tutorials/monolith_kinetics`

Reference

1. G. Schaub, D. Unruh, J. Wang, and T. Turek, "Kinetic analysis of selective catalytic NOx reduction (SCR) in a catalytic filter," *Chemical Engineering and Processing*, vol. 42, no. 3, pp. 365–371, 2003.

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 **0D**.

2 In the **Select Physics** tree, select **Chemical Species Transport>Reaction Engineering (re)**.

3 Click **Add**.

4 Click **Study**.

5 In the **Select Study** tree, select **Preset Studies for Selected Physics Interfaces> Stationary Plug Flow**.

6 Click **Done**.

GLOBAL DEFINITIONS

Parameters 1

Start by reading in a set of global parameters defining the process conditions for the monolith reactor, including the dimensions of the reactive channels, the flow rate of the reacting gas, and the temperature conditions.

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 `monolith_kinetics_parameters.txt`.

DEFINITIONS

Variables 1

1 In the **Model Builder** window, under **Component 1 (comp1)** right-click **Definitions** and choose **Variables**.

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

3 In the table, enter the following settings:

Name	Expression	Unit	Description
S	re.r_1/re.r_2		Selectivity
a	a0*exp(-E0/(R_const*re.T))	m³/mol	Concentration correction

REACTION ENGINEERING (RE)

Next, create a Thermodynamic System that includes all thermodynamic properties (such as enthalpy, entropy, and so on) needed in the simulation of the reacting system. The thermodynamic properties are automatically coupled to the Reaction Engineering interface.

In the **Reaction Engineering** 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 **oxygen (7782-44-7, O2)**.

3 Click **Add Selected**.

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

5 Click **Add Selected**.

6 In the **Species** list, select **nitrogen oxide (10102-43-9, NO)**.

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 **ammonia (7664-41-7, H3N)**.

11 Click + **Add Selected**.

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

SELECT THERMODYNAMIC MODEL

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

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

REACTION ENGINEERING (RE)

Now define the chemical reactions. First, type in the reaction formula for NO reduction. The **Reaction** will automatically interpret the reaction formula and suggest reaction rates based on the mass action law.

Reaction 1

1 In the **Model Builder** window, under **Component 1 (comp1)** right-click **Reaction Engineering (re)** and choose **Reaction**.

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

3 In the **Formula** text field, type `4NO+4NH3+O2=>4N2+6H2O`.

Notice that, there being several ways to balance this formula, the button **Balance** is not applicable in this case.

In this example, replace the automatically generated **reaction rate** expression with the rate expression known from the literature. Use the **max operator** in the denominator of the rate expression to avoid negative concentrations.

4 Locate the **Reaction Rate** section. From the list, choose **User defined**.

5 In the r_j text field, type `re.kf_1*re.c_NO*a*re.c_NH3/(1+a*max(re.c_NH3, 0[M]))`.

In the next step, update the reaction order.

6 Find the **Volumetric overall reaction order** subsection. In the **Forward** text field, type `1`.

7 Locate the **Rate Constants** section. Select the **Use Arrhenius expressions** check box.

8 In the A^{f} text field, type `A1`.

9 In the E^{f} text field, type `E1`.

In the same fashion, now define the reaction for NH_3 oxidation.

Reaction 2

1 In the **Reaction Engineering** toolbar, click **Reaction**.

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

3 In the **Formula** text field, type `NH3+O2=>N2+H2O`.

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

This reaction can be balanced with **Balance** since there is only one solution to the balancing problem.

5 Locate the **Reaction Rate** section. From the list, choose **User defined**.

6 In the r_j text field, type `re.kf_2*re.c_NH3`.

Continue by updating the reaction order so that it matches with the rate expression.

7 Find the **Volumetric overall reaction order** subsection. In the **Forward** text field, type `1`.

8 Locate the **Rate Constants** section. Select the **Use Arrhenius expressions** check box.

9 In the A^{f} text field, type `A2`.

10 In the E^{f} text field, type `E2`.

Now choose reactor type.

11 In the **Model Builder** window, click **Reaction Engineering (re)**.

12 In the **Settings** window for **Reaction Engineering**, locate the **Reactor** section.

13 From the **Reactor type** list, choose **Plug flow**.

Couple all species in **Reaction Engineering** to corresponding species in the created **Thermodynamic System**.

14 Locate the **Mixture Properties** section. Select the **Thermodynamics** check box.

15 Locate the **Species Matching** section. In the table, enter the following settings:

Species	From Thermodynamics
H2O	H2O
N2	N2
NH3	H3N
NO	NO
O2	O2

Isolate the effect of temperature and reactant ratios by keeping the volumetric flow rate constant. Therefore, select to compute pressure from the ideal gas law.

16 Locate the **Mixture Properties** section. From the **Reactor pressure** list, choose **Ideal gas law**.

The following steps allow you to study the reaction rate for fixed reactant concentrations, solely as a function of temperature. First, use the independent variable `V` (reactor volume, written `re.Vr`) to set up a temperature ramp between 500 K and

750 K. Then, after defining initial values, lock the concentrations of reactant NO and NH_3 and add a **Parametric sweep** feature.

17 Locate the **Energy Balance** section. From the list, choose **Exclude**.

18 In the *T* text field, type `500[K]+250[K/m^3]*re.Vr`.

19 Locate the **Reactor** section. Find the **Mass balance** subsection. In the *v* text field, type `vrate`.

Initial Values 1

Enter the initial values.

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

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

3 In the table, enter the following settings:

Species	Molar flow rate (mol/s)
H2O	F_H2O_in
N2	F_N2_in
NH3	F_NH3_in
NO	F_NO_in
O2	F_O2_in

Lock the reactant concentrations in the following way.

Species: NO

1 In the **Model Builder** window, click **Species: NO**.

2 In the **Settings** window for **Species**, click to expand the **Species Concentration/Activity** section.

3 Select the **Constant concentration/activity** check box.

Species: NH3

1 In the **Model Builder** window, click **Species: NH3**.

2 In the **Settings** window for **Species**, locate the **Species Concentration/Activity** section.

3 Select the **Constant concentration/activity** check box.

Now add a **Parametric Sweep** feature to solve the model for a set of NH_3:NO ratios.

STUDY 1

Parametric Sweep

1 In the **Study** toolbar, click **Parametric Sweep**.

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

3 Click **Add**.

4 From the list in the **Parameter name** column, choose **X0 (Ratio NH3 to NO at inlet)**.

5 Click **Range**.

6 In the **Range** dialog box, type `1` in the **Start** text field.

7 In the **Step** text field, type `0.2`.

8 In the **Stop** text field, type `2`.

9 Click **Replace**.

Solution 1 (sol1)

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

It is good practice to tighten the default solver tolerances and make sure that the solution plots do not change between consecutive test runs. Both the relative and absolute tolerance should be tightened. In this case the relative tolerance needs to be reduced to 10^{-7}.

Step 1: Stationary Plug Flow

1 In the **Model Builder** window, click **Step 1: Stationary Plug Flow**.

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

3 From the **Tolerance** list, choose **User controlled**.

4 In the **Relative tolerance** text field, type `1e-7`.

5 In the **Study** toolbar, click **Compute**.

All the solutions generated by pressing **Compute** in the **Study** interface are saved and can be copied and modified. This enable easy postprocessing of the results, since several different case studies, within the same study, can be saved and compared.

Parametric Solutions 1 (sol2)

In the **Model Builder** window, right-click **Parametric Solutions 1 (sol2)** and choose **Solution> Copy**.

Kinetics

1 In the **Model Builder** window, under **Study 1>Solver Configurations** click **Parametric Solutions 1 - Copy 1 (sol9)**.

2 In the **Settings** window for **Solution**, type `Kinetics` in the **Label** text field.

Create the plots shown in Figure 1 and Figure 2 by following the steps below.

RESULTS

Reaction rate

1 In the **Model Builder** window, under **Results** click **Molar Flow Rate (re)**.

2 In the **Settings** window for **1D Plot Group**, type `Reaction rate` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Study 1/Kinetics (sol9)**.

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

5 Locate the **Plot Settings** section. In the **x-axis label** text field, type `Temperature (K)`.

6 Locate the **Legend** section. From the **Position** list, choose **Upper left**.

Global 1

1 In the **Model Builder** window, expand the **Reaction rate** node, then click **Global 1**.

2 In the **Settings** window for **Global**, click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)> Reaction Engineering>re.r_1 - Reaction rate - mol/(m³·s)**.

3 Locate the **x-Axis Data** section. From the **Parameter** list, choose **Expression**.

4 In the **Expression** text field, type `re.T`.

5 Click to expand the **Coloring and Style** section. In the **Width** text field, type `2`.

6 Click to expand the **Legends** section. Find the **Include** subsection. Clear the **Expression** check box.

7 In the **Reaction rate** toolbar, click  **Plot**.

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

Selectivity

1 In the **Model Builder** window, right-click **Reaction rate** and choose **Duplicate**.

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

3 Locate the **Legend** section. From the **Position** list, choose **Upper right**.

Global 1

1 In the **Model Builder** window, expand the **Selectivity** node, then click **Global 1**.

2 In the **Settings** window for **Global**, click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)>Definitions> Variables>S - Selectivity**.

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

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

Figure 1 and Figure 2 are now done. Let's continue by setting up a proper reactor model where the effect of generated heat, as well as consumption of reactants, can be studied.

REACTION ENGINEERING (RE)

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Reaction Engineering (re)**.

2 In the **Settings** window for **Reaction Engineering**, locate the **Energy Balance** section.

3 From the list, choose **Include**.

4 In the Q text field, type `(T_amb-re.T)*UA`.

Initial Values 1

1 In the **Model Builder** window, under **Component 1 (comp1)>Reaction Engineering (re)** click **Initial Values 1**.

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

3 In the $T_{0,\text{in}}$ text field, type `T_in`.

Species: NO

1 In the **Model Builder** window, click **Species: NO**.

2 In the **Settings** window for **Species**, locate the **Species Concentration/Activity** section.

3 Clear the **Constant concentration/activity** check box.

Species: NH3

1 In the **Model Builder** window, click **Species: NH3**.

2 In the **Settings** window for **Species**, locate the **Species Concentration/Activity** section.

3 Clear the **Constant concentration/activity** check box.

STUDY 1

Step 1: Stationary Plug Flow

Enter the volumes to solve for, from zero to total reactor volume.

1 In the **Model Builder** window, under **Study 1** click **Step 1: Stationary Plug Flow**.

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

3 In the **Output volumes** text field, type `0[m^3] L*A`.

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

Parametric Solutions 1 (sol2)

In the **Model Builder** window, right-click **Parametric Solutions 1 (sol2)** and choose **Solution> Copy**.

Nonisothermal

1 In the **Model Builder** window, under **Study 1>Solver Configurations** click **Parametric Solutions 1 - Copy 1 (sol22)**.

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

The following steps generate Figure 3.

RESULTS

Molar flow rate NH3, Nonisothermal

1 In the **Model Builder** window, under **Results** click **Molar Flow Rate (re)**.

2 In the **Settings** window for **1D Plot Group**, type `Molar flow rate NH3, Nonisothermal` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Study 1/Nonisothermal (sol22)**.

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

5 Locate the **Plot Settings** section. Select the **y-axis label** check box.

6 In the associated text field, type `Molar flow rate NH<sub>3</sub> (mol/s)`.

Global 1

1 In the **Model Builder** window, expand the **Molar flow rate NH3, Nonisothermal** node, then click **Global 1**.

2 In the **Settings** window for **Global**, click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)> Reaction Engineering>re.F_NH3 - Molar flow rate - mol/s**.

3 Locate the **Coloring and Style** section. In the **Width** text field, type `2`.

4 Locate the **Legends** section. Find the **Include** subsection. Clear the **Expression** check box.

5 In the **Molar flow rate NH3, Nonisothermal** toolbar, click **Plot**.

STUDY 1

Parametric Sweep

1 In the **Model Builder** window, under **Study 1** click **Parametric Sweep**.

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

3 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
X0 (Ratio NH3 to NO at inlet)	`range(1.3,0.1,1.5)`	

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

Parametric Solutions 1 (sol2)

In the **Model Builder** window, right-click **Parametric Solutions 1 (sol2)** and choose **Solution>Copy**.

Nonisothermal 2

1 In the **Model Builder** window, under **Study 1>Solver Configurations** click **Parametric Solutions 1 - Copy 1 (sol32)**.

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

The following instructions generate Figure 4.

RESULTS

Selectivity, Nonisothermal

1 In the **Model Builder** window, under **Results** click **Temperature (re)**.

2 In the **Settings** window for **1D Plot Group**, type `Selectivity, Nonisothermal` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Study 1/Nonisothermal 2 (sol32)**.

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

5 Locate the **Legend** section. From the **Position** list, choose **Middle right**.

Global 1

1 In the **Model Builder** window, expand the **Selectivity, Nonisothermal** node, then click **Global 1**.

2 In the **Settings** window for **Global**, click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)>Definitions>Variables>S - Selectivity**.

3 Locate the **Coloring and Style** section. In the **Width** text field, type `2`.

4 Locate the **Legends** section. Find the **Include** subsection. Clear the **Expression** check box.

5 In the **Selectivity, Nonisothermal** toolbar, click **Plot**.

The following instructions generate Figure 5.

Temperature, Nonisothermal

1 In the **Model Builder** window, right-click **Selectivity, Nonisothermal** and choose **Duplicate**.

2 In the **Settings** window for **1D Plot Group**, type `Temperature, Nonisothermal` in the **Label** text field.

Global 1

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

2 In the **Settings** window for **Global**, click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)> Reaction Engineering>re.T - Temperature - K**.

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

Graph Marker 1

1 Right-click **Global 1** and choose **Graph Marker**.

2 In the **Settings** window for **Graph Marker**, locate the **Display** section.

3 From the **Display** list, choose **Max**.

4 Locate the **Text Format** section. In the **Display precision** text field, type `3`.

5 Select the **Include unit** check box.

Global 2

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

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

3 Click **Clear Table**.

4 In the table, enter the following settings:

Expression	Unit	Description
`(F_NO_in/vrate-re.c_NO)/(F_NO_in/vrate)`	1	`Conversion`

Graph Marker 1

1 In the **Model Builder** window, expand the **Global 2** node, then click **Graph Marker 1**.

2 In the **Settings** window for **Graph Marker**, locate the **Text Format** section.

3 Clear the **Include unit** check box.

4 Click to expand the **Coloring and Style** section. From the **Anchor point** list, choose **Lower right**.

Temperature, Nonisothermal

1 In the **Model Builder** window, click **Temperature, Nonisothermal**.

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

3 From the **Parameter selection (X0)** list, choose **From list**.

4 In the **Parameter values (X0)** list, choose **1.3** and **1.5**.

5 Locate the **Plot Settings** section. Select the **Two y-axes** check box.

6 In the table, select the **Plot on secondary y-axis** check box for **Global 2**.

7 In the **Temperature, Nonisothermal** toolbar, click **Plot**.

Global 2

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

2 In the **Settings** window for **Global**, locate the **Coloring and Style** section.

3 From the **Color** list, choose **Cycle (reset)**.

4 Find the **Line style** subsection. From the **Line** list, choose **Dashed**.