



# Analysis of NO<sub>x</sub> Reaction Kinetics

## Introduction

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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  $\text{NH}_3$  is present in amounts that do not limit the NO reduction reaction. At the same time, excess  $\text{NH}_3$  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.

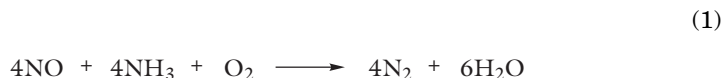
This tutorial aims at getting a primary understanding of the monolithic reactor. It concentrates on the investigation of the selectivity of the reactions by solving the model with the Plug Flow ideal reactor type in the Reaction Engineering interface.

## Model Definition

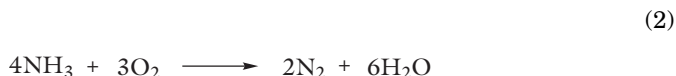
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### CHEMICAL REACTIONS

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



However, ammonia can at the same time undergo oxidation:



The heterogeneous catalytic conversion of NO to  $\text{N}_2$  is described by an Eley-Rideal mechanism. A key reaction step involves the reaction of gas-phase NO with surface-adsorbed  $\text{NH}_3$ . The following rate equation (SI unit:  $\text{mol}/(\text{m}^3 \cdot \text{s})$ ) has been suggested in [Ref. 1](#) for [Equation 1](#):

$$r_1 = k_1 c_{\text{NO}} \frac{a c_{\text{NH}_3}}{1 + a c_{\text{NH}_3}}$$

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<sup>3</sup>·s)) is given by

$$r_2 = k_2 c_{\text{NH}_3} \quad (3)$$

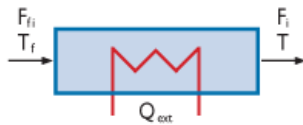
where

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

The competing chemical reactions raise the issue of optimal dosing of NH<sub>3</sub> to handle the reduction process. Stoichiometry suggests a 1:1 ratio of NH<sub>3</sub> to NO as a lower limit. It is likely that a stoichiometric excess of NH<sub>3</sub> is necessary but, at the same time, we want to avoid unnecessarily high levels of NH<sub>3</sub> in the gas stream leaving the catalytic converter.

#### SINGLE CHANNEL MODEL

To find the minimal level of NH<sub>3</sub> 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:

$$\frac{dF_i}{dV} = R_i \quad (4)$$

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

$$F_i = vc_i \quad (5)$$

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<sup>2</sup>):

$$v = uA \quad (6)$$

The energy balance for the ideal reacting gas is:

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

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

The model is first solved with [Equation 4](#), [Equation 5](#), and [Equation 6](#) for several different ratios of reactant concentrations (NH<sub>3</sub>:NO) and with a temperature ramp along the reactor. The molar flow rates of NH<sub>3</sub> 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

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### REACTION KINETICS ANALYSIS

Analyzing the kinetics can help narrow down a proper NH<sub>3</sub>:NO ratio. A first study looks at the reaction rates of the reduction and oxidation reactions, for fixed molar flow rates of

$\text{NH}_3$  and  $\text{NO}$ , 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  $\text{NH}_3$ : $\text{NO}$  ratios ( $X0$ ) ranging from 1 to 2. The concentration of  $\text{NO}$  in the exhaust gas entering the catalytic converter is known to be  $0.0411 \text{ mol/m}^3$ .

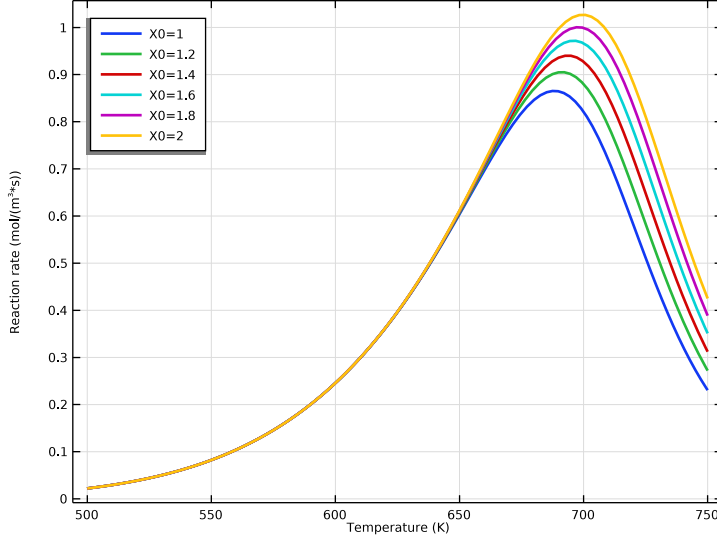


Figure 1: Reaction rates of the  $\text{NO}$  reduction reaction ( $r_1$ ) as a function of temperature. The  $\text{NH}_3$ : $\text{NO}$  ratio ranges from 1 to 2 and the molar flow rates of  $\text{NH}_3$  and  $\text{NO}$  are kept constant throughout the reactor.

The rate of  $\text{NO}$  reduction goes through a maximum and falls off at higher temperatures. The maximum shifts toward higher temperatures as the ratio  $\text{NH}_3$ : $\text{NO}$  increases. This behavior is explained by the desorption rate of  $\text{NH}_3$  from the catalyst surface becoming faster than the reaction of adsorbed  $\text{NH}_3$  with gas-phase  $\text{NO}$ .

According to Equation 3, the oxidation rate increases with increased temperature and  $\text{NH}_3$  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.

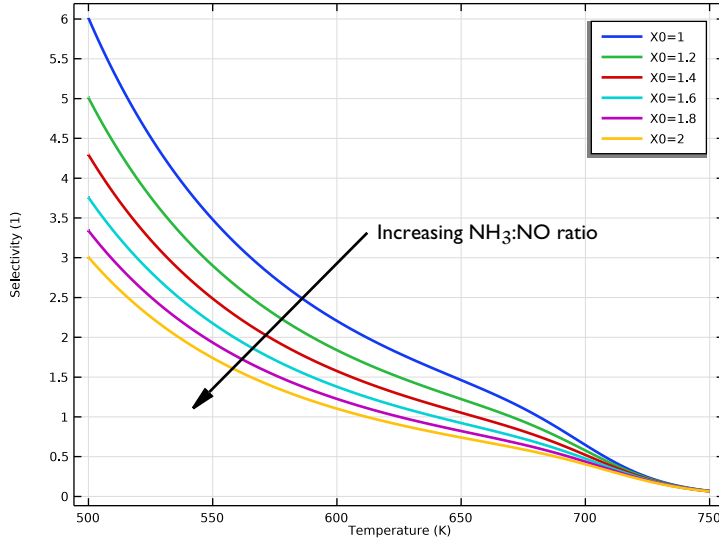


Figure 2: Selectivity parameter ( $r_1/r_2$ ) as a function of temperature. The  $\text{NH}_3:\text{NO}$  ratio ranges from 1 to 2.

The kinetic analysis suggests that preferred working conditions involve moderate temperatures and relatively low ratios of  $\text{NH}_3:\text{NO}$ .

#### SINGLE CHANNEL MODEL

To find the minimal level of  $\text{NH}_3$  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  $41.1 \text{ mmol/m}^3$  of NO, with a temperature of 523 K, passing through the monolith at 0.3 m/s, the plug-flow model suggests a  $\text{NH}_3:\text{NO}$  ratio higher than 1.2 to guarantee that  $\text{NH}_3$  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  $45\text{e-}5\text{ m}^3$ .

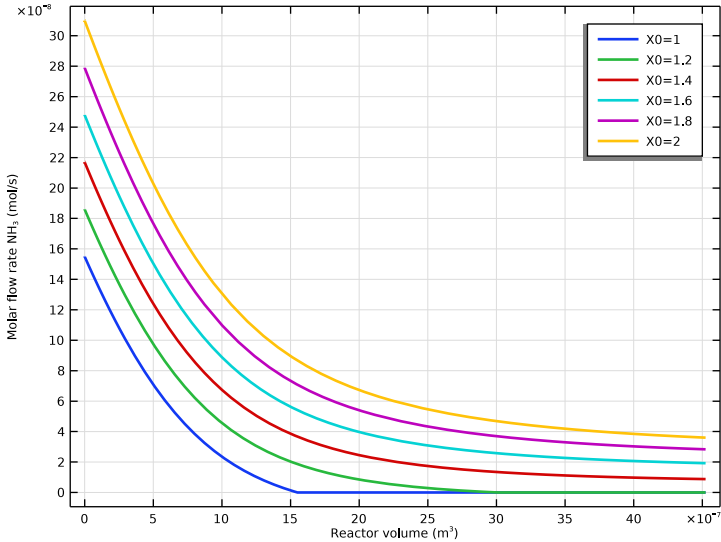


Figure 3: Molar flow rate of  $\text{NH}_3$  as function of channel volume.

A plot of the selectivity parameter (Figure 4) confirms that the NO reduction chemistry is favored in the monolith reactor at  $\text{NH}_3\text{:NO}$  ratios ranging from 1.3 to 1.5.

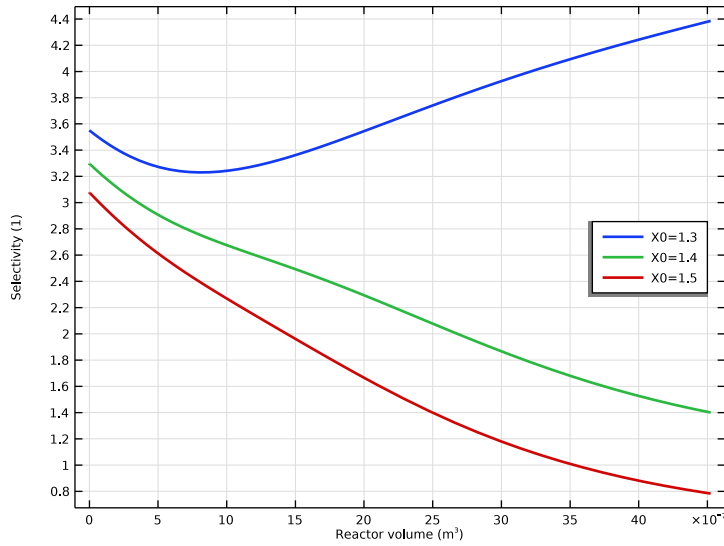
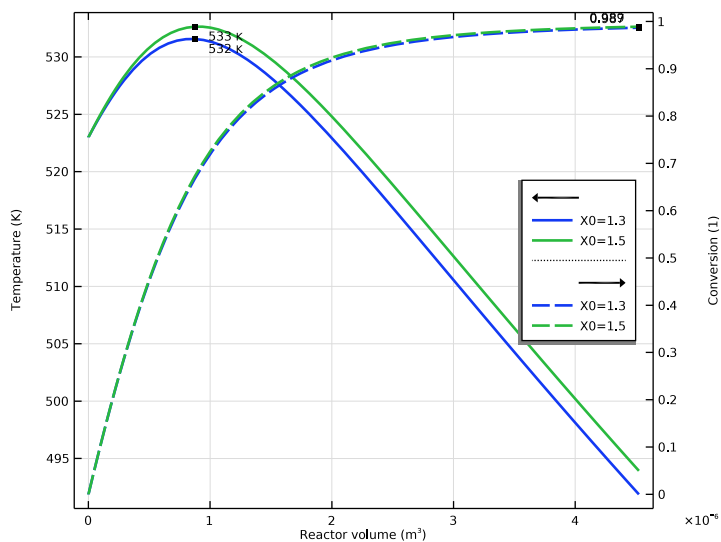


Figure 4: Selectivity parameter ( $r_1/r_2$ ) as a function of channel volume. The  $\text{NH}_3:\text{NO}$  ratio ranges from 1.3 to 1.5.

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  $\text{NH}_3$ . 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  $\text{NH}_3\text{:NO}$  ratio between 1.3 and 1.4 appears appropriate for the 3D model.

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**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.

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**Application Library path:** `Chemical_Reaction_Engineering_Module/Tutorials/monolith_kinetics`

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## Reference

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I. G. Schaub, D. Unruh, J. Wang, and T. Turek, “Kinetic analysis of selective catalytic NO<sub>x</sub> reduction (SCR) in a catalytic filter,” *Chemical Engineering and Processing*, vol. 42, no. 3, pp. 365–371, 2003.

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**Note:** This model is included in the booklet *Introduction to the Chemical Reaction Engineering Module*.


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## Modeling Instructions




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

### NEW

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


### MODEL WIZARD

- 1 In the **Model Wizard** window, click  **OD**.
- 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 I*

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 I**.
- 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 I*

- 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	$a_0 \cdot \exp(-E_0/(R_{const} \cdot re.T))$	m <sup>3</sup> /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  $4\text{NO} + 4\text{NH}_3 + \text{O}_2 \Rightarrow 4\text{N}_2 + 6\text{H}_2\text{O}$ .

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  $\text{re.kf}_1 * \text{re.c\_NO} * a * \text{re.c\_NH}_3 / (1 + a * \max(\text{re.c\_NH}_3, 0[\text{M}]))$ .

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  $\text{NH}_3$  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  $\text{NH}_3 + \text{O}_2 \Rightarrow \text{N}_2 + \text{H}_2\text{O}$ .

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  $\text{re.kf}_2 \cdot \text{re.c}_{\text{NH}_3}$ .

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  $A_2$ .

10 In the  $E^f$  text field, type  $E_2$ .

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
H <sub>2</sub> O	H <sub>2</sub> O
N <sub>2</sub>	N <sub>2</sub>
NH <sub>3</sub>	H <sub>3</sub> N
NO	NO
O <sub>2</sub>	O <sub>2</sub>

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  $\text{NH}_3$  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 I*

Enter the initial values.

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

**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 **Constant Concentration/Activity** section.

**3** Select the **Keep concentration/activity constant** check box.

#### *Species: NH3*

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




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

**3** Select the **Keep concentration/activity constant** check box.

Now add a **Parametric Sweep** feature to solve the model for a set of  $\text{NH}_3$ :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, under **Study 1** 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  $1\text{e-}7$ .
- 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, under **Study 1>Solver Configurations** 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 **ID 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 I*

- 1 In the **Model Builder** window, expand the **Reaction rate** node, then click **Global I**.
- 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\_I - Reaction rate - mol/(m<sup>3</sup>·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. From the **Width** list, choose **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 **ID Plot Group**, type Selectivity in the **Label** text field.
- 3 Locate the **Legend** section. From the **Position** list, choose **Upper right**.

### *Global I*

- 1 In the **Model Builder** window, expand the **Selectivity** node, then click **Global I**.
- 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 us 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  $(T_{\text{amb}} - re.T) * UA$ .

#### *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  $T_{\text{in}}$ .

#### *Species: NO*

- 1 In the **Model Builder** window, click **Species: NO**.
- 2 In the **Settings** window for **Species**, locate the **Constant Concentration/Activity** section.
- 3 Clear the **Keep concentration/activity constant** check box.


#### *Species: NH3*

- 1 In the **Model Builder** window, click **Species: NH3**.
- 2 In the **Settings** window for **Species**, locate the **Constant Concentration/Activity** section.
- 3 Clear the **Keep concentration/activity constant** 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  $0[m^3] \quad L * A$ .
- 4 In the **Home** toolbar, click  **Compute**.

### *Parametric Solutions I (sol2)*

In the **Model Builder** window, under **Study I>Solver Configurations** right-click **Parametric Solutions I (sol2)** and choose **Solution>Copy**.

### *Nonisothermal*

- 1 In the **Model Builder** window, under **Study I>Solver Configurations** click **Parametric Solutions I - Copy I (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 NH<sub>3</sub>, Nonisothermal*

- 1 In the **Model Builder** window, under **Results** click **Molar Flow Rate (re)**.
- 2 In the **Settings** window for **ID Plot Group**, type Molar flow rate NH<sub>3</sub>, Nonisothermal in the **Label** text field.
- 3 Locate the **Data** section. From the **Dataset** list, choose **Study I/Nonisothermal (sol22)**.
- 4 Locate the **Title** section. From the **Title type** list, choose **None**.
- 5 Locate the **Plot Settings** section.
- 6 Select the **y-axis label** check box. In the associated text field, type Molar flow rate NH<sub>3</sub> (mol/s).

### *Global I*

- 1 In the **Model Builder** window, expand the **Molar flow rate NH<sub>3</sub>, Nonisothermal** node, then click **Global I**.
- 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 I (comp1)>Reaction Engineering>re.F\_NH3 - Molar flow rate - mol/s**.
- 3 Locate the **Coloring and Style** section. From the **Width** list, choose **2**.
- 4 Locate the **Legends** section. Find the **Include** subsection. Clear the **Expression** check box.
- 5 In the **Molar flow rate NH<sub>3</sub>, Nonisothermal** toolbar, click  **Plot**.

## **STUDY I**

### *Parametric Sweep*

- 1 In the **Model Builder** window, under **Study I** 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, under **Study 1>Solver Configurations** 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 **ID 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. From the **Width** list, choose **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 **ID 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, under **Results** click **Temperature, Nonisothermal**.

- 2 In the **Settings** window for **ID Plot Group**, locate the **Data** section.
- 3 From the **Parameter selection (X0)** list, choose **From list**.
- 4 In the **Parameter values (X0)** list, choose **I.3** and **I.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**.

