



Model created in COMSOL Multiphysics 6.4

Analysis of NO_x and Ammonia Conversion Kinetics in a Dual-Bed Plug-Flow Reactor

Introduction

This example looks at the reduction of harmful nitrogen oxides NO_x (NO and NO₂) into nitrogen in an exhaust gas after-treatment system of a heavy-duty diesel truck. The nitrogen oxides are reduced by ammonia that is injected upstream of the after-treatment system consisting of a catalytic, monolithic reactor.

The reactor has two catalytic beds with two different catalysts. The upstream bed is a selective catalytic reduction (SCR) bed with the purpose of selectively convert NO_x to nitrogen. The second bed is an ammonia-slip-catalyst (ASC). This bed should convert the remaining ammonia to nitrogen.

The dosing rate of ammonia has a direct influence on the conversion of NO_x. Too low dosing rate leads to exhaust of unconverted nitrogen oxides, while too much ammonia may give ammonia-slip, or even NO_x emissions, since a side reaction in the ammonia-slip bed is formation of NO_x from ammonia. Since the engine load affects the exhaust gas temperature, the volumetric flow rate of exhaust gas, as well as the concentration of former nitrogen oxide, the dosing needs to be dynamically adjusted.

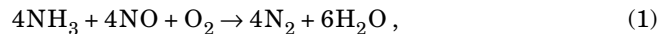
This tutorial aims at getting a primary understanding of the chemical kinetics in the dual-bed reactor. This is achieved by solving the model with the Plug Flow ideal reactor type in the Reaction Engineering interface. The influence of temperature, volumetric flow rate, and ammonia-to-NO_x ratio is investigated.

Model Definition

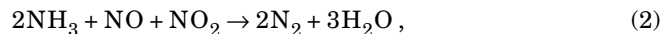
CHEMICAL REACTIONS

In this tutorial model, a simplified reaction setup is used with six reactions in the first bed, and four reactions in the second bed.

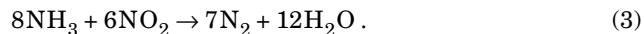
In the selective catalytic reduction bed, there are three desired SCR reactions that take place. These are the so called standard SCR reaction



the fast SCR reaction



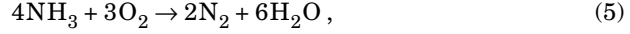
and the NO₂ SCR reaction



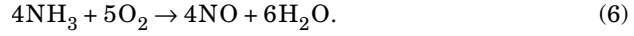
There is also the oxidation of nitrogen monoxide into nitrogen dioxide



Finally, there are also two undesired reactions present. It is the oxidation of ammonia into nitrogen



and the oxidation of ammonia into nitrogen oxide



Except for the homogeneous gas phase equilibrium reaction (4), all reactions are heterogeneous catalytic reactions with reaction rates that depend on surface coverage. The surface coverage of ammonia can be related to the fluid phase concentration by assuming that ammonia desorption and adsorption are in equilibrium. With a Langmuir-Hinshelwood mechanism, based on this assumption, global rate expressions can be derived. The following five rate expressions have been suggested in [Ref. 1](#):

$$r_1 = k_1 \frac{c_{\text{NO}} c_{\text{O}_2} c_{\text{NH}_3}}{(1 + K_{\text{NH}_3} c_{\text{NH}_3})}.$$

Here, K_{NH_3} is the ammonia adsorption equilibrium constant, expressed with the pre-exponential factor $K_{\text{NH}_3, 523}$, and the adsorption enthalpy ΔH_{ads} :

$$K_{\text{NH}_3} = K_{\text{NH}_3, 523} \exp\left(\frac{-\Delta H_{\text{ads}}}{R} \left(\frac{1}{523} - \frac{1}{T}\right)\right).$$

The rate expression for the fast SCR reaction is

$$r_2 = k_2 \frac{c_{\text{NO}_2} c_{\text{NO}} c_{\text{NH}_3}}{(1 + K_{\text{NH}_3} c_{\text{NH}_3})}.$$

Correspondingly, the rate expression for the NO_2 -SCR reaction is

$$r_3 = k_3 \frac{c_{\text{NO}_2} c_{\text{NH}_3}}{(1 + K_{\text{NH}_3} c_{\text{NH}_3})}.$$

The equilibrium rate expression follows the mass action law, giving the forward rate

$$r_{4, f} = k_4 c_{\text{NO}}^2 c_{\text{O}_2} - r_{4, r} c_{\text{NO}_2}^2.$$

The reversed reaction rate is derived from the forward reaction rate and the equilibrium constant K_{eq} that is derived from thermodynamics laws:

$$r_{4,r} = \frac{r_{4,f}}{K_{\text{eq}}}.$$

The reaction rate expression for the undesired oxidation of ammonia into nitrogen is defined as

$$r_5 = k_5 \frac{c_{\text{NH}_3} c_{\text{O}_2}}{(1 + K_{\text{NH}_3} c_{\text{NH}_3})}.$$

The reaction rate for the undesired oxidation of ammonia into nitrogen monoxide also follows a Langmuir–Hinshelwood mechanism, and has been suggested to take this form (Ref. 2):

$$r_6 = k_6 \frac{c_{\text{NH}_3} c_{\text{O}_2}}{G}.$$

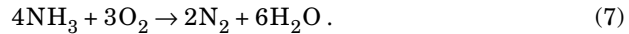
Here, G is a variable that accounts for the inhibition effects caused by adsorption of other species on the surface:

$$G = T(1 + K_1 c_{\text{NO}} + K_2 c_{\text{H}_2\text{O}})^2 (1 + K_3 c_{\text{NH}_3})^2 (1 + K_4 c_{\text{O}_2})^2,$$

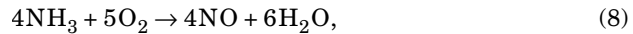
where K_i ($i = 1, \dots, 4$) follows an Arrhenius-type expression

$$K_i = A_i \exp\left(\frac{-E_i}{RT}\right).$$

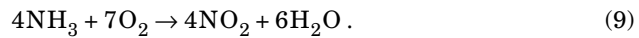
In the ammonia slip catalyst bed, there is one desired, two undesired reactions, and Reaction 4, the homogeneous equilibrium, that take place. The desired reaction is the oxidation of ammonia to form nitrogen:



The two undesired reactions are the oxidation of ammonia into nitrogen monoxide



and the oxidation of ammonia into nitrogen dioxide



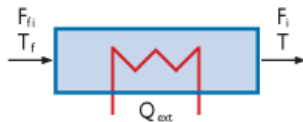
Reactions 7 and 8 are the same chemical equations as Reactions 5 and 6, but since the catalyst is different, the kinetic parameters differ. The rate expressions are assumed the same though. The rate expression for Reaction 9 is

$$r_9 = k_9 \frac{c_{\text{NH}_3} c_{\text{O}_2}}{G} .$$

The competing chemical reactions raise the issue of optimal dosing of NH_3 to handle the reduction process in the first bed. Stoichiometry suggests a 1:1 ratio of NH_3 to NO as a lower limit for the standard SCR reaction. Due to the undesired oxidation of ammonia it is likely that a stoichiometric excess of NH_3 is necessary. The excess ammonia will be converted in the second ammonia-slip catalyst bed. The NO_x forming side reactions in the second bed motivates as low ammonia injection as possible. This is also important for economic and pressure-drop reasons.

SINGLE CHANNEL MODEL

To find the lowest level of NH_3 required to reduce the NO_x present in the exhaust gas, a reactor model accounting for changing reactant compositions and system temperature is needed. 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

$$\frac{dF_i}{dV} = R_i \quad (10)$$

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: $\text{mol}/(\text{m}^3 \cdot \text{s})$). The molar flow

rate is related to the species concentrations, c_i (SI unit: mol/m³), through the volumetric flow rate, v (SI unit: m³/s):

$$F_i = v c_i \quad (11)$$

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: m²):

$$v = uA \quad (12)$$

The energy balance for the ideal reacting gas is

$$\sum_i F_i C_{p,i} \frac{dT}{dV} = Q_{\text{ext}} + Q \quad (13)$$

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/(m³·s)). Q denotes the heat due to chemical reaction (SI unit: J/(m³·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/(m³·s)). The Q_{ext} is set to zero, based on the assumption that the modeled channel is close to the center of the monolith, and that the reactor is well insulated.

In this model, several different aspects of the system is studied. First, the temperature operating window for the selective catalytic reduction bed, is investigated. This is achieved by solving Equation 10–Equation 13 for a range of inlet temperatures, keeping the ammonia-to-NOx ratio (ANR) equal to 1.3 at the inlet. A value of 1.3 is chosen since more than stoichiometric amounts of ammonia is needed.

Thereafter, the ammonia-to-NOx ratio is varied together with the inlet temperature. This results in an understanding of how the system responds to these two parameters.

As a third step, the ammonia-slip-catalyst is added to the study and the influence of ammonia-to-NOx is investigated. Except for the varied ANR, the inlet conditions are kept constant.

In reality, depending on the engine load, the exhaust gas properties vary significantly. Therefore, as the last step, the ammonia-to-NOx ratio is kept constant, while the inlet conditions are varied between three engine load cases; high load, intermediate load, and low load. This will reveal if the ammonia-to-NOx ratio should be varied with engine load.

TEMPERATURE OPERATING WINDOW

The first study aimed at finding the operating window for the selective catalytic reduction catalyst. This was achieved by varying the inlet gas temperature, while keeping the $\text{NH}_3:\text{NO}_x$ ratio equal to 1.3. The resulting NO_x conversion along the reactor axis as a function of inlet temperature is seen in Figure 1.

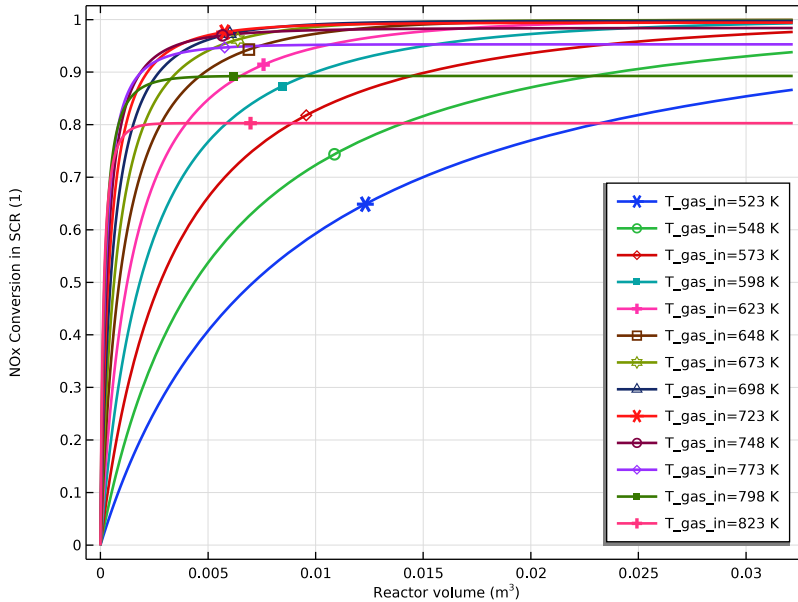


Figure 1: NO_x conversion along the reactor axis as a function of inlet temperature, for an $\text{NH}_3:\text{NO}_x$ ratio equal to 1.3, in the selective catalytic reduction bed.

The conversion increases more rapidly for higher inlet temperatures, but around 600 K the conversion starts to decrease due to the competing oxidation of ammonia with oxygen.

Figure 2 shows the temperature increase in the first bed along the reactor axis. The exothermic reactions create a temperature increase. For the four highest temperatures the

outlet temperature has decreased. This is a result of the different selectivity in the system at different temperatures.

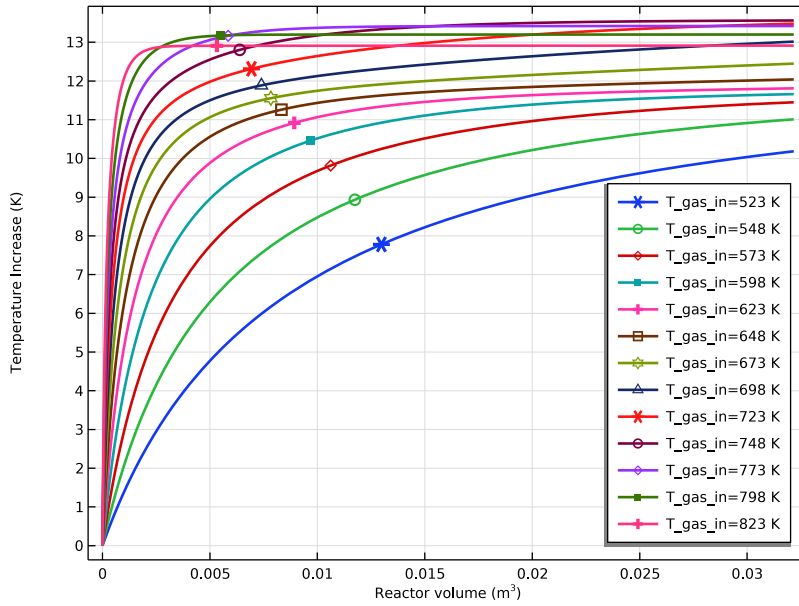


Figure 2: Temperature along the reactor axis as a function of inlet temperature in the selective catalytic reduction bed. $\text{NH}_3:\text{NO}_x$ ratio equal to 1.3

The optimal temperature operating window, defined as the temperatures giving maximum conversion of NO_x, is 620–720K for the SCR bed at an NH₃:NO_x ratio equal to 1.3. The conversion of NO_x is close to complete at this temperature. This is seen in [Figure 3](#).

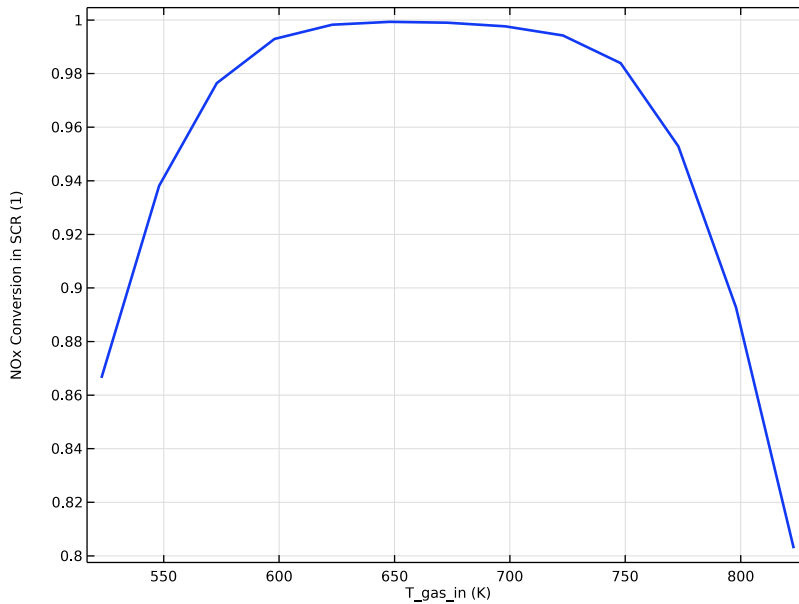


Figure 3: Final conversion of NO_x in the selective catalytic reduction (SCR) bed as a function of inlet gas temperature. The NH₃:NO_x ratio is equal to 1.3.

INFLUENCE OF TEMPERATURE AND NH₃:NO_x RATIO

Moving on to investigate the influence of both inlet temperature and ammonia-to-NO_x ratio (ANR). [Figure 4](#) shows that for an increased ANR, the operating window widens and

shifts toward lower temperatures. In addition, the conversion of NO_x increases for the investigated range.

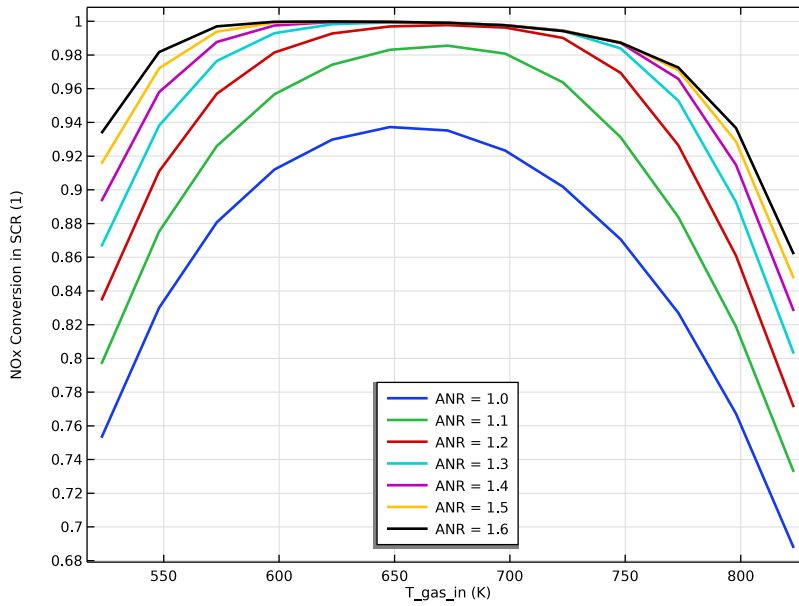


Figure 4: Final conversion of NO_x in the selective catalytic reduction (SCR) bed as a function of inlet gas temperature and NH₃:NO_x ratio.

The conversion of ammonia as a function of ANR and inlet gas temperature is seen in Figure 5. Complete conversion of ammonia is reached for all ANR at inlet gas temperatures above 750 K.

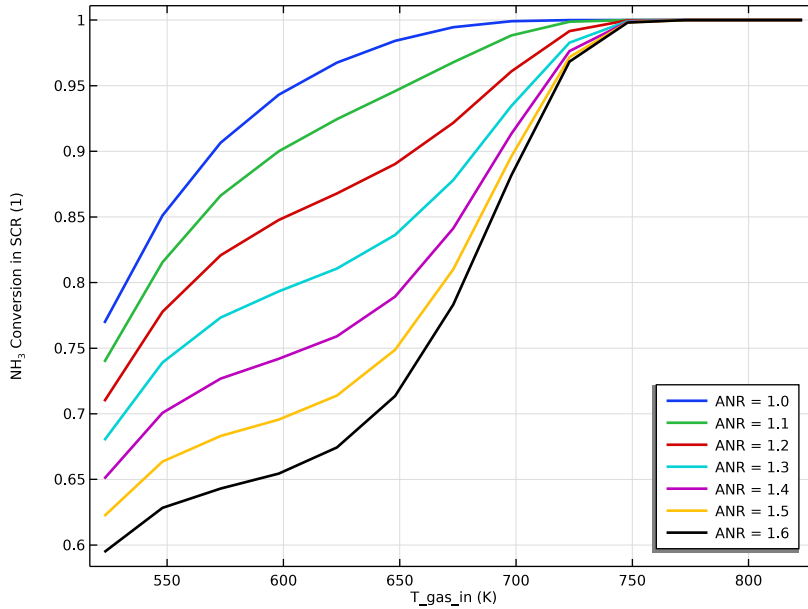


Figure 5: Final conversion of ammonia in the selective catalytic reduction (SCR) bed as a function of inlet gas temperature and $\text{NH}_3:\text{NO}_x$ ratio.

DUAL-BED MODEL

The results from the single bed model revealed that the optimal conversion window for NOx is at a lower temperature than that of ammonia. We also saw that the ammonia-to-NOx ratio needs to be kept above 1.2 to reach complete conversion of NOx. Higher ammonia dosing gives more ammonia-slip. With an ammonia slip catalyst downstream of the first bed, the excess ammonia can be converted. This allows for higher ANR. The

influence of ANR in the dual bed system is therefore investigated. Figure 6 shows the molar fraction of ammonia and NOx along a single monolith channel in each bed,

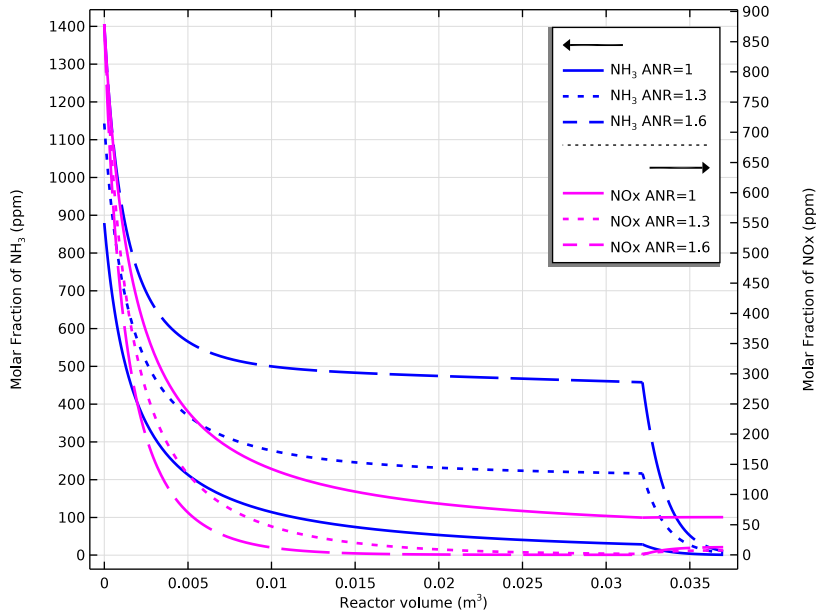


Figure 6: Molar fraction of ammonia and NOx in the dual bed system along the reactor axis. The $\text{NH}_3:\text{NOx}$ ratio varies from 1 to 1.6.

The molar fractions decrease rapidly early in the SCR catalyst bed, and for the highest ammonia concentration the conversion of NOx is complete halfway through the first bed. The unconverted ammonia is almost completely converted in the ASC bed, even for the highest dosing, but due to undesired side reactions in the ASC bed, the NOx concentration increases. Even though the conversion is close to complete, the molar

fractions might still be too high to pass the emission standards. The conversion in the dual bed system is seen in Figure 7.

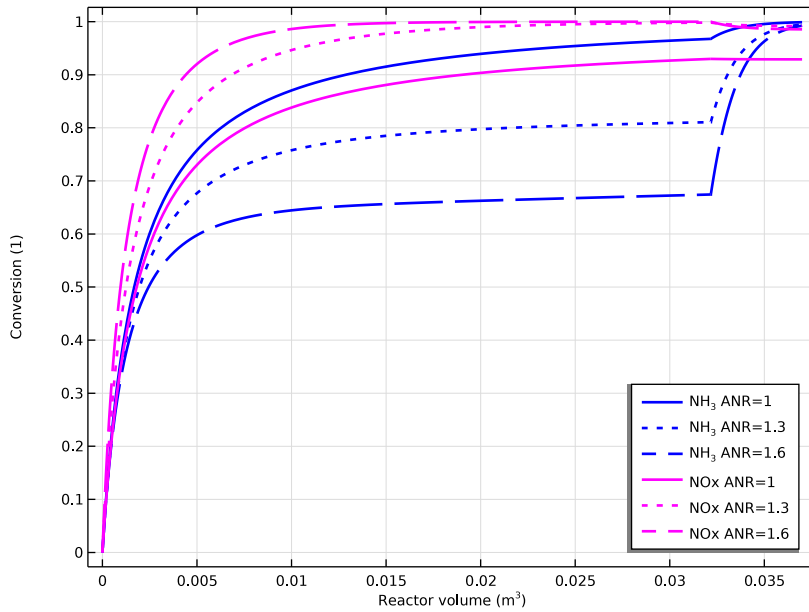


Figure 7: Conversion of ammonia and NOx in the dual bed system along the reactor axis. The NH₃:NOx ratio varies from 1 to 1.6.

The results this far have revealed that both temperature and the ammonia-to-NOx ratio are important factors to consider. Additionally, the ANR should be kept as low as possible, even though the system contains an ammonia-slip catalyst bed.

In a real application, the engine load of the truck will affect the exhaust gas temperature, the composition of the exhaust gas, and the volumetric flow. Therefore, the last part of this model studies three engine load cases. The three engine load cases result in the following inlet gas conditions:

TABLE I: INLET GAS CONDITIONS FOR EACH ENGINE LOAD CASE STUDIED.

	Low Load	Intermediate load	High load
Temperature	523 K	623 K	703 K
Molar fraction of NO	300 ppm	800 ppm	1300 ppm
Mass flow rate	0.086 kg/s	0.110 kg/s	0.160 kg/s

High engine load gives more NO_x, higher gas flow rate, and higher temperature. The previous studies were all performed for an intermediate engine load. A low engine load will result in low flow rate, low gas temperature, but low NO_x from the engine. Figure 8 shows the molar fraction for these three load cases, and an ANR of 1.3.

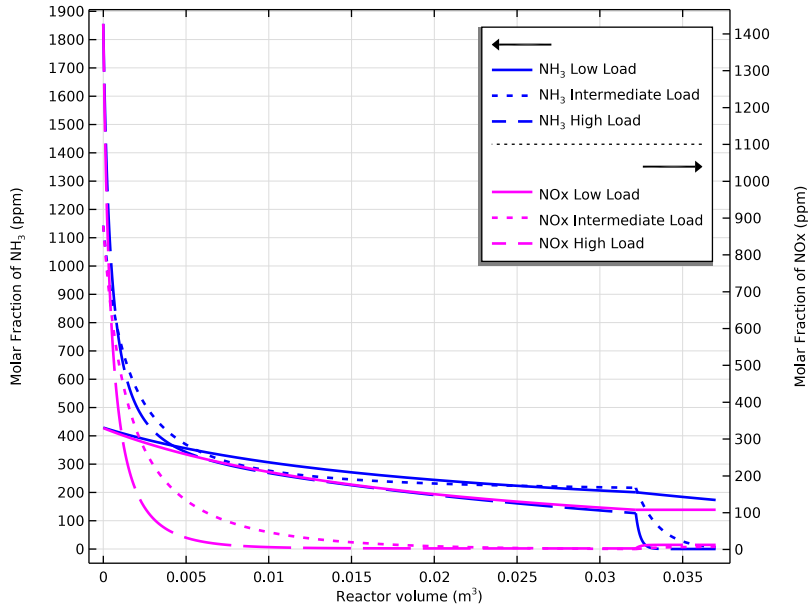


Figure 8: Molar fraction of NO_x and ammonia as a function of axis position in the reactor. ANR equals 1.3, and the results from the three engine load cases are shown.

This figure reveals that the highest emissions of both NO_x and ammonia result from the lowest engine load. This is a result of the low temperature, which decreases the reaction rate. Even though the incoming gas contains the lowest amount of NO_x to start with, and the flow rate of gas is the lowest, the reaction rate is simply too low. This is also seen in Figure 3.

The lowest NO_x emission is achieved for the intermediate load. The high load would give lower NO_x emissions if the ANR is decreased, as some of the NO_x out from the reactor results from ammonia oxidation in the ASC-bed. For the intermediate engine load the ASC-catalyst volume should be increased, and perhaps the ANR increased.

Figure 9 shows the conversion in the dual bed system for each of the three engine load cases.

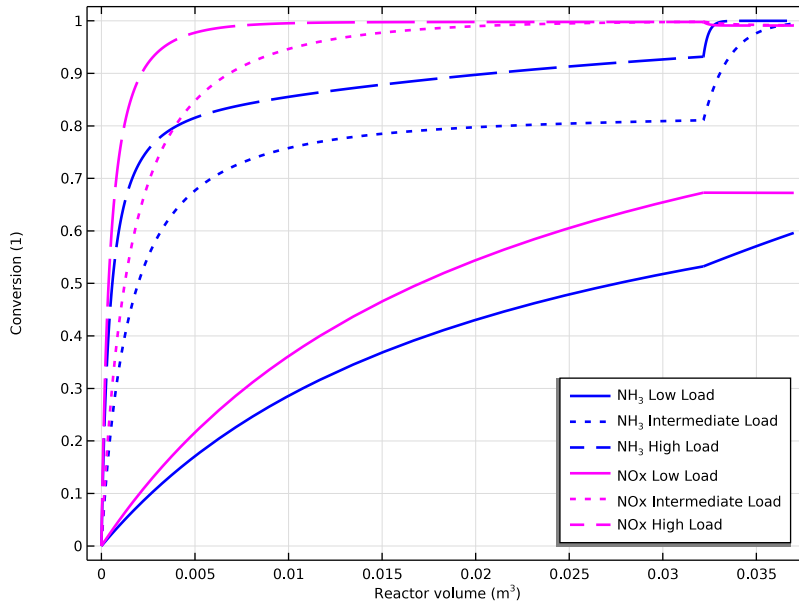


Figure 9: Conversion of ammonia and NOx for the three engine load cases and an ANR equal to 1.3.

The single channel model with two beds have been modeled as adiabatic, assuming that the modeled channel is close to the monolith center, and that the reactor is well insulated.

Figure 10 shows the temperature increase along the reactor for each of the three engine load cases.

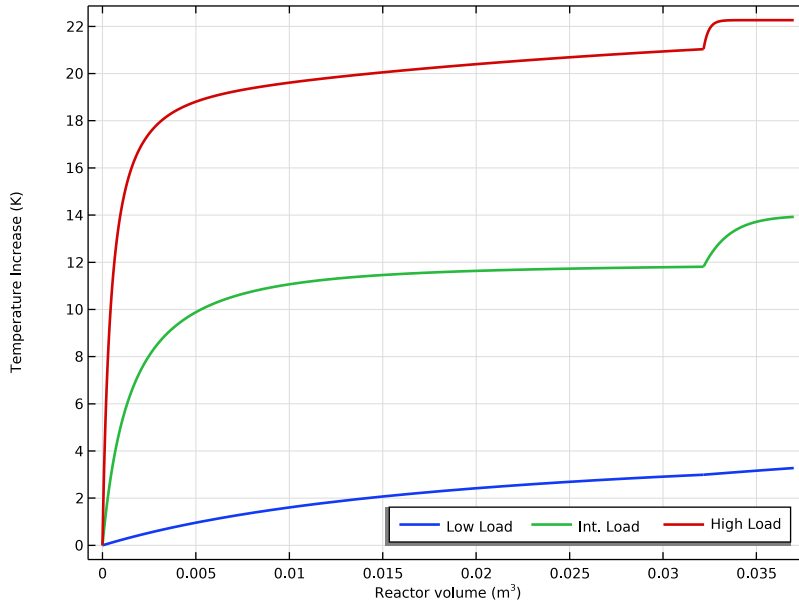


Figure 10: Temperature increase in the reactor for the three engine load cases and an ANR equal to 1.3.

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 space-dependent reactor model accounting for this variation is called for. Based on the single channel model simulations, a $\text{NH}_3:\text{NO}_x$ ratio of 1.3 appears appropriate for the extended model.

Note: For details on the extended space-dependent model of the reactor, see the example [NO_x and Ammonia Conversion in a Dual-Bed Monolithic Reactor](#) in the Chemical Reaction Engineering Module Application Library.

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

References


1. U. De-La-Torre, B. Pereda-Ayo, M.A. Gutiérrez-Ortiz, J.A. González-Marcos, and J.R. González-Velasco, “Steady-state NH₃-SCR global model and kinetic parameter estimation for NO_x removal in diesel engine exhaust aftertreatment with Cu/chabazite,” *Catalysis Today*, vol. 296, pp. 95–104, 2017.
2. B.K. Yun, M.Y. Kim, “Modeling the selective catalytic reduction of NO_x by ammonia over a Vanadia-based catalyst from heavy duty diesel exhaust gases,” *Appl. Therm. Eng.*, vol. 50, pp. 152–158, 2013.

Application Library path: Chemical_Reaction_Engineering_Module/Tutorials/monolith_kinetics




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  **Next**.
- 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: Engine Load Cases

Start by reading in a set of global parameters that will be used when setting up this model. The parameter files contain process conditions for different engine loads, kinetic parameters, and catalyst dimensions.

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_engine_load_cases_parameters.txt`.

The loaded file contains mass flow rates, nitrogen monoxide molar fraction, and temperature of the exhaust gas entering the reactor. Low engine load gives a lower mass flow rate, lower temperature, and less nitrogen oxides, than a high engine load.

Rename the parameter node and add a **Parameter Case**.

5 In the **Label** text field, type `Parameters: Engine Load Cases`.

Use the global feature **Parameter Case** to specify the load cases to be used later in **Parametric Sweep**.


Cases

1 In the **Home** toolbar, click  **Parameters** and choose **Add > Parameters**.

2 In the **Settings** window for **Parameters**, type `Cases` in the **Label** text field.

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


Name	Expression	Value	Description
m	m2	0.11 kg/s	Mass flow rate (case 2 is default)
y	y2	8E-4	NO molar fraction (case 2 is default)
T	T2	623 K	Inlet temperature (case 2 is default)

4 In the **Home** toolbar, click  **Parameter Case**.


5 In the **Settings** window for **Case**, type `Low Load` in the **Label** text field.

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

Name	Expression	Description
m	m1	Mass flow rate (case 2 is default)
y	y1	NO molar fraction (case 2 is default)
T	T1	Inlet temperature (case 2 is default)

7 In the **Home** toolbar, click  **Parameter Case**.

8 In the **Settings** window for **Case**, type `Intermediate Load` in the **Label** text field.

9 In the **Home** toolbar, click  **Parameter Case**.



10 In the **Settings** window for **Case**, type High Load in the **Label** text field.

11 Locate the **Parameters** section. In the table, enter the following settings:



Name	Expression	Description
m	m3	Mass flow rate (case 2 is default)
y	y3	NO molar fraction (case 2 is default)
T	T3	Inlet temperature (case 2 is default)

Load some more parameter files.



Parameters: Temperature and Monolith Parameters

- 1 In the **Home** toolbar, click  **Parameters** and choose **Add > Parameters**.
- 2 In the **Settings** window for **Parameters**, type Parameters: Temperature and Monolith Parameters in the **Label** text field.
- 3 Locate the **Parameters** section. Click  **Load from File**.
- 4 Browse to the model's Application Libraries folder and double-click the file monolith_kinetics_temperature_monolith_parameters.txt.

Parameters: Flow and Composition

- 1 In the **Home** toolbar, click  **Parameters** and choose **Add > Parameters**.
- 2 In the **Settings** window for **Parameters**, type Parameters: Flow and Composition in the **Label** text field.
- 3 Locate the **Parameters** section. Click  **Load from File**.
- 4 Browse to the model's Application Libraries folder and double-click the file monolith_kinetics_flow_composition_parameters.txt.

Parameters: Reaction Kinetics


- 1 In the **Home** toolbar, click  **Parameters** and choose **Add > Parameters**.
- 2 In the **Settings** window for **Parameters**, type Parameters: Reaction Kinetics in the **Label** text field.
- 3 Locate the **Parameters** section. Click  **Load from File**.
- 4 Browse to the model's Application Libraries folder and double-click the file monolith_kinetics_kinetic_parameters.txt.

Load some variable files. These are, compared to parameters, not constant in value. We will add expressions for reaction rate constants, that vary with composition and

temperature. For your convenience, we load the expressions from a file, but you can also type them in directly in the table.

DEFINITIONS


Variables: Reaction Kinetics SCR

- 1 In the **Model Builder** window, under **Component 1 (comp1)** right-click **Definitions** and choose **Variables**.
- 2 In the **Settings** window for **Variables**, type Variables: Reaction Kinetics SCR in the **Label** text field.
- 3 Locate the **Variables** section. Click  **Load from File**.
- 4 Browse to the model's Application Libraries folder and double-click the file `monolith_kinetics_SCR_kinetics_variables.txt`.
Since the reactions have not yet been added to the model, the expression for G is shown with a yellow underline, indicating unknown variables.

Variables: Reaction Kinetics ASC

- 1 In the **Model Builder** window, right-click **Definitions** and choose **Variables**.
- 2 In the **Settings** window for **Variables**, type Variables: Reaction Kinetics ASC in the **Label** text field.
- 3 Locate the **Variables** section. Click the **Load** button. From the menu, choose **Load from File**.
- 4 Browse to the model's Application Libraries folder and double-click the file `monolith_kinetics_ASC_kinetics_variables.txt`.

Variables: Postprocessing

- 1 Right-click **Definitions** and choose **Variables**.
- 2 In the **Settings** window for **Variables**, type Variables: Postprocessing in the **Label** text field.
- 3 Locate the **Variables** section. Click  **Load from File**.
- 4 Browse to the model's Application Libraries folder and double-click the file `monolith_kinetics_postprocessing_variables.txt`.


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. One of the species in the system, NO₂, is not part of the built-in

thermodynamics database, and it must be added as a **User-Defined Species**. This species has been added to another application library model. Load it from there.


GLOBAL DEFINITIONS

Gas System 1 (pp1)

- 1 In the **Reaction Engineering** 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`.

Remove the species N_2O_4 since it is not needed, then add the rest of the species for this model.

Species 1 (N2O4)

- 1 In the **Model Builder** window, expand the **Global Definitions > Thermodynamics > User-Defined Species** node.
- 2 Right-click **Species 1 (N2O4)** and choose **Delete**.
- 3 In the **Reaction Engineering** toolbar, click  **Thermodynamics** and choose **Thermodynamic System**.

SELECT SYSTEM

- 1 Go to the **Select System** window.
- 2 Click the **Next** button in the window toolbar.

SELECT SPECIES

- 1 Go to the **Select Species** window.
- 2 From the **Database** list, choose **User defined**.
- 3 In the **Species** list box, select **NO2 (10102-44-0, NO2)**.
- 4 Click **+ Add Selected**.
- 5 From the **Database** list, choose **COMSOL**.
- 6 In the **Species** list box, select **ammonia (7664-41-7, H3N)**.
- 7 Click **+ Add Selected**.
- 8 In the **Species** list box, select **nitrogen (7727-37-9, N2)**.
- 9 Click **+ Add Selected**.
- 10 In the **Species** list box, select **nitrogen oxide (10102-43-9, NO)**.
- 11 Click **+ Add Selected**.

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

13 Click **+ Add Selected**.

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

15 Click **+ Add Selected**.

16 Click the **Next** button in the window toolbar.

SELECT THERMODYNAMIC MODEL

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

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

GLOBAL DEFINITIONS


Gas System 1 (pp1)

This example studies a catalytic reactor containing two monolithic catalysts placed in series. The first one is the selective catalytic reduction (SCR) catalyst. This catalyst should convert NO and NO₂ into N₂ by reducing it with ammonia. There are side reactions though, consuming ammonia without converting NO_x (NO + NO₂). More than stoichiometric amounts of ammonia must therefore be fed. Downstream of the SCR catalyst, an ammonia slip catalyst (ASC) is installed, with the purpose of oxidizing the ammonia to nitrogen. Also here there are undesired side reactions. Begin by defining the chemical reactions in the first catalyst.

REACTION ENGINEERING (RE)

First, type in the global reaction formula for the standard SCR reaction. The **Reaction** will automatically interpret the reaction formula and suggest reaction rates based on the mass action law.

(1) *Standard SCR: 4 NH₃ + 4 NO + O₂ => 4 N₂ + 6 H₂O*

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 4NH₃+4NO+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. The variable K_NH₃ is defined in a **Variables** feature.

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

5 In the r_j text field, type $re.kf_1*re.c_{NO}*re.c_{O2}*re.c_{NH3}/(1+K_{NH3}*re.c_{NH3})$.

In the next step, update the reaction order for this global reaction rate expression.

6 Locate the **Reaction Orders** section. Find the **Volumetric overall reaction order** subsection. In the **Forward** text field, type 3.

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

8 In the A^f text field, type A1_SCR.


9 In the E^f text field, type E1_SCR.

Finally, edit the label of the **Reaction** feature. This is optional.

10 In the **Label** text field, type (1) Standard SCR: $4 NH_3 + 4 NO + O_2 \Rightarrow 4 N_2 + 6 H_2O$.

In the same fashion, now define the reactions for the fast SCR reaction, the NO_2 SCR reaction, the oxidation of NO, and the two undesired NH_3 consuming reactions.

(2) Fast SCR: $2 NH_3 + NO + NO_2 \Rightarrow 2 N_2 + 3 H_2O$

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 $2 NH_3 + NO + NO_2 \Rightarrow 2 N_2 + 3 H_2O$.

4 In the **Label** text field, type (2) Fast SCR: $2 NH_3 + NO + NO_2 \Rightarrow 2 N_2 + 3 H_2O$.

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

6 In the r_j text field, type $re.kf_2*re.c_{NO2}*re.c_{NO}*re.c_{NH3}/(1+K_{NH3}*re.c_{NH3})$.

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

8 In the A^f text field, type A2_SCR.

9 In the E^f text field, type E2_SCR.

10 Locate the **Reaction Orders** section. Find the **Volumetric overall reaction order** subsection. In the **Forward** text field, type 3.

(3) NO_2 SCR: $8 NH_3 + 6 NO_2 \Rightarrow 7 N_2 + 12 H_2O$

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 $8 NH_3 + 6 NO_2 \Rightarrow 7 N_2 + 12 H_2O$.

4 In the **Label** text field, type (3) NO_2 SCR: $8 NH_3 + 6 NO_2 \Rightarrow 7 N_2 + 12 H_2O$.

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

- 6 In the r_j text field, type $re.kf_3*re.c_NO2*re.c_NH3 / (1+K_NH3*re.c_NH3)$.
- 7 Locate the **Rate Constants** section. Select the **Use Arrhenius expressions** checkbox.
- 8 In the A^f text field, type A3_SCR.
- 9 In the E^f text field, type E3_SCR.
- 10 Locate the **Reaction Orders** section. Find the **Volumetric overall reaction order** subsection. In the **Forward** text field, type 2.

(4) *Equilibrium: 2 NO + O2 <=> 2 NO2*

- 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 $2\ NO + O2 \rightleftharpoons 2\ NO2$.
- 4 In the **Label** text field, type (4) Equilibrium: 2 NO + O2 <=> 2 NO2.
- 5 Locate the **Rate Constants** section. Select the **Specify equilibrium constant** checkbox.
- 6 Select the **Use Arrhenius expressions** checkbox.
- 7 In the A^f text field, type A4.
- 8 In the E^f text field, type E4.

We want to derive the equilibrium constant from thermodynamics, which means that we first need to connect (couple) the species in **Reaction Engineering** to those in the **Thermodynamic System**.


By adding these reactions, the required **Species** features have been added. Couple all species in **Reaction Engineering** to corresponding species in the created **Thermodynamic System**.

- 9 In the **Model Builder** window, click **Reaction Engineering (re)**.
- 10 In the **Settings** window for **Reaction Engineering**, locate the **Mixture Properties** section.
- 11 Select the **Thermodynamics** checkbox.
- 12 Locate the **Species Matching** section. In the table, enter the following settings:


Species	From Thermodynamics
H2O	H2O
N2	N2
NH3	H3N
NO	NO
NO2	NO2
O2	O2

Now, **Reaction Engineering** is coupled to the **Thermodynamic System**, and the equilibrium constant for the fourth reaction is derived from thermodynamics. Continue to add the final two reactions.

(5) *Undesired Oxidation: 4 NH₃ + 3 O₂ => 2 N₂ + 6 H₂O*

- 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 4 NH₃ + 3 O₂ => 2 N₂ + 6 H₂O.
- 4 In the **Label** text field, type (5) Undesired Oxidation: 4 NH₃ + 3 O₂ => 2 N₂ + 6 H₂O.
- 5 Locate the **Reaction Rate** section. From the list, choose **User defined**.
- 6 In the r_j text field, type $re.kf_5*(re.c_NH3*re.c_O2)/(1+K_NH3*re.c_NH3)$.
- 7 Locate the **Rate Constants** section. Select the **Use Arrhenius expressions** checkbox.
- 8 In the A^f text field, type A5_SCR.
- 9 In the E^f text field, type E5_SCR.
- 10 Locate the **Reaction Orders** section. Find the **Volumetric overall reaction order** subsection. In the **Forward** text field, type 2.

(6) *Undesired NO Formation: 4 NH₃ + 5 O₂ => 4 NO + 6 H₂O*

- 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 4 NH₃ + 5 O₂ => 4 NO + 6 H₂O.
- 4 In the **Label** text field, type (6) Undesired NO Formation: 4 NH₃ + 5 O₂ => 4 NO + 6 H₂O.
- 5 Locate the **Reaction Rate** section. From the list, choose **User defined**.
- 6 In the r_j text field, type $re.kf_6*re.c_O2*re.c_NH3/G$.
- 7 Locate the **Rate Constants** section. Select the **Use Arrhenius expressions** checkbox.
- 8 In the A^f text field, type A6_SCR.
- 9 In the E^f text field, type E6_SCR.
- 10 Locate the **Reaction Orders** section. Find the **Volumetric overall reaction order** subsection. In the **Forward** text field, type 2.

Now choose reactor type, and rename the interface to something descriptive.

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

12 In the **Settings** window for **Reaction Engineering**, type Selective Catalytic Reduction Catalyst (SCR) in the **Label** text field.

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

Continue by defining the initial values for the reactor. Use the parameters previously loaded from files.

Initial Values I

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

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

3 In the $T_{0,in}$ text field, type T_{gas_in} .

4 Locate the **Volumetric Species Initial Values** section. In the table, enter the following settings:

Species	Molar flow rate (mol/s)
H2O	FH2O_in
N2	FN2_in
NH3	FNH3_in
NO	FNO_in
NO2	FN02_in
O2	F02_in

Add a second **Reaction Engineering** physics interface to define the ammonia slip catalyst.

ADD PHYSICS

1 In the **Home** toolbar, click  **Add Physics** to open the **Add Physics** window.

2 Go to the **Add Physics** window.

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

4 Click the **Add to Component I** button in the window toolbar.

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

AMMONIA SLIP CATALYST (ASC)


1 In the **Settings** window for **Reaction Engineering**, type Ammonia Slip Catalyst (ASC) in the **Label** text field.

2 Locate the **Reactor** section. From the **Reactor type** list, choose **Plug flow**.


3 Locate the **Energy Balance** section. From the **Energy balance** list, choose **Include**.

Add the reactions.


(1) *Desired NH3 Oxidation: 4 NH3 + 3 O2 => 2 N2 + 6 H2O*

- 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 $4 \text{ NH}_3 + 3 \text{ O}_2 \Rightarrow 2 \text{ N}_2 + 6 \text{ H}_2\text{O}$.
- 4 In the **Label** text field, type (1) Desired NH3 Oxidation: $4 \text{ NH}_3 + 3 \text{ O}_2 \Rightarrow 2 \text{ N}_2 + 6 \text{ H}_2\text{O}$.
- 5 Locate the **Reaction Rate** section. From the list, choose **User defined**.
- 6 In the r_j text field, type $\text{re2.kf}_1 \cdot \text{re2.c}_{\text{NH}_3} \cdot \text{re2.c}_{\text{O}_2} / (1 + \text{K}_{\text{NH}_3_ASC} \cdot \text{re2.c}_{\text{NH}_3})$.
- 7 Locate the **Rate Constants** section. Select the **Use Arrhenius expressions** checkbox.
- 8 In the A^f text field, type A1_ASC.
- 9 In the E^f text field, type E1_ASC.
- 10 Locate the **Reaction Orders** section. Find the **Volumetric overall reaction order** subsection. In the **Forward** text field, type 2.

(2) *Undesired NO Formation: 4 NH3 + 5 O2 => 4 NO + 6 H2O*


- 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 $4 \text{ NH}_3 + 5 \text{ O}_2 \Rightarrow 4 \text{ NO} + 6 \text{ H}_2\text{O}$.
- 4 In the **Label** text field, type (2) Undesired NO Formation: $4 \text{ NH}_3 + 5 \text{ O}_2 \Rightarrow 4 \text{ NO} + 6 \text{ H}_2\text{O}$.
- 5 Locate the **Reaction Rate** section. From the list, choose **User defined**.
- 6 In the r_j text field, type $\text{re2.kf}_2 \cdot \text{re2.c}_{\text{O}_2} \cdot \text{re2.c}_{\text{NH}_3} / \text{G_ASC}$.
- 7 Locate the **Rate Constants** section. Select the **Use Arrhenius expressions** checkbox.
- 8 In the A^f text field, type A2_ASC.
- 9 In the E^f text field, type E2_ASC.
- 10 Locate the **Reaction Orders** section. Find the **Volumetric overall reaction order** subsection. In the **Forward** text field, type 2.

(3) *Equilibrium: 2 NO + O2 <=> 2 NO2*

- 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 $2 \text{ NO} + \text{O}_2 \Leftrightarrow 2 \text{ NO}_2$.
- 4 In the **Label** text field, type (3) Equilibrium: $2 \text{ NO} + \text{O}_2 \Leftrightarrow 2 \text{ NO}_2$.

- 5 Locate the **Rate Constants** section. Select the **Specify equilibrium constant** checkbox.
- 6 Select the **Use Arrhenius expressions** checkbox.
- 7 In the A^f text field, type A4.
- 8 In the E^f text field, type E4.

(4) *Undesired NO2 Formation: 4 NH3 + 7 O2 => 4 NO2 + 6 H2O*

- 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 4 NH3 + 7 O2 => 4 NO2 + 6 H2O.
- 4 In the **Label** text field, type (4) Undesired NO2 Formation: 4 NH3 + 7 O2 => 4 NO2 + 6 H2O.
- 5 Locate the **Reaction Rate** section. From the list, choose **User defined**.
- 6 In the r_j text field, type $re2.kf_4*re2.c_NH3*re2.c_O2/G_ASC$.
- 7 Locate the **Rate Constants** section. Select the **Use Arrhenius expressions** checkbox.
- 8 In the A^f text field, type A4_ASC.
- 9 In the E^f text field, type E4_ASC.
- 10 Locate the **Reaction Orders** section. Find the **Volumetric overall reaction order** subsection. In the **Forward** text field, type 2.

Couple the interface to the **Thermodynamics System** and edit the volumetric flow rate and the reactor pressure.

- 11 In the **Model Builder** window, click **Ammonia Slip Catalyst (ASC) (re2)**.
- 12 In the **Settings** window for **Reaction Engineering**, locate the **Mixture Properties** section.
- 13 Select the **Thermodynamics** checkbox.
- 14 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

Define the initial condition for the system. The gas entering the ammonia slip catalyst is that exiting the upstream SCR catalyst. Use **Ctrl+Space** in the text field to see a list of valid inputs, for example the variable names defined by the SCR system.

Initial Values I

- 1 In the **Model Builder** window, click **Initial Values I**.
- 2 In the **Settings** window for **Initial Values**, locate the **General Parameters** section.
- 3 In the $T_{0,in}$ text field, type $re.T$.
- 4 Locate the **Volumetric Species Initial Values** section. In the table, enter the following settings:

Species	Molar flow rate (mol/s)
H2O	$re.F_{H2O}$
N2	$re.F_{N2}$
NH3	$re.F_{NH3}$
NO	$re.F_{NO}$
NO2	$re.F_{NO2}$
O2	$re.F_{O2}$

Now, investigate the temperature operating window for the first part of the reactor, the SCR catalyst. Investigate this by varying the temperature of the inlet exhaust gas using **Auxiliary Sweep**. The Ammonia to NO_x Ratio (ANR) is set to 1.3 (see **Parameters: Flow and Composition**) and the mass flow rate of exhaust gas corresponds to engine load case 2, that is, intermediate engine speed.

STUDY I

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 I** 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 $0 \ V_{SCR}$.
- 4 Locate the **Physics and Variables Selection** section. In the **Solve for** column of the table, under **Component 1 (comp1)**, clear the checkbox for **Ammonia Slip Catalyst (ASC) (re2)**.
- 5 Click to expand the **Study Extensions** section. Select the **Auxiliary sweep** checkbox.
- 6 Click **+ Add**.
- 7 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
$T_{gas,in}$ (Temperature of inlet exhaust gas)	range (523, 25, 825)	K

It is good practice to check the default scales for the dependent variables set up by the study. These are found under the **Solver Configurations** node. For this case, using scales based on the initial values improves the convergence rate and the solution accuracy.

Solution 1 (sol1)

- 1 In the **Study** toolbar, click  **Show Default Solver**.
- 2 In the **Model Builder** window, expand the **Solution 1 (sol1)** node, then click **Dependent Variables 1**.
- 3 In the **Settings** window for **Dependent Variables**, locate the **Scaling** section.
- 4 From the **Method** list, choose **Initial-value based**.
Rename the study into something descriptive, and compute.
- 5 In the **Model Builder** window, click **Study 1**.
- 6 In the **Settings** window for **Study**, type Study 1: SCR Temperature Operating Window, ANR = 1.3, Case 2 in the **Label** text field.
- 7 In the **Study** toolbar, click  **Compute**.


RESULTS

Conversion Along Reactor Axis

Take a look at the resulting default plots. Modify them and follow the below steps to create [Figure 1](#), [Figure 2](#), and [Figure 3](#).



- 1 In the **Settings** window for **ID Plot Group**, type Conversion Along Reactor Axis in the **Label** text field.
- 2 Click to expand the **Title** section. From the **Title type** list, choose **None**.
- 3 Locate the **Legend** section. From the **Position** list, choose **Lower right**.

Global 1

- 1 In the **Model Builder** window, expand the **Conversion Along Reactor Axis** node, then click **Global 1**.
- 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
X_NOx_SCR	1	NOx Conversion in SCR

- 5 Click to expand the **Coloring and Style** section. From the **Color cycle** list, choose **Long**.

- 6 From the **Width** list, choose **2**.
- 7 Find the **Line markers** subsection. From the **Marker** list, choose **Cycle**.
- 8 In the **Number** text field, type 1.
- 9 Click to expand the **Legends** section. Find the **Include** subsection. Clear the **Expression** checkbox.
- 10 Click the  **Zoom Extents** button in the **Graphics** toolbar.
- 11 In the **Conversion Along Reactor Axis** toolbar, click  **Plot**.

Temperature (re)

In the **Model Builder** window, under **Results** right-click **Temperature (re)** and choose **Delete**.



Temperature Increase Along Reactor Axis

- 1 In the **Model Builder** window, right-click **Conversion Along Reactor Axis** and choose **Duplicate**.
- 2 In the **Model Builder** window, click **Conversion Along Reactor Axis 1**.
- 3 In the **Settings** window for **ID Plot Group**, type Temperature Increase Along Reactor Axis in the **Label** text field.


Global 1

- 1 In the **Model Builder** window, click **Global 1**.
- 2 In the **Settings** window for **Global**, locate the **y-Axis Data** section.
- 3 In the table, enter the following settings:

Expression	Unit	Description
re.T-T_gas_in	K	Temperature Increase

- 4 Click the  **Zoom Extents** button in the **Graphics** toolbar.
- 5 In the **Temperature Increase Along Reactor Axis** toolbar, click  **Plot**.

Temperature Operating Window

- 1 In the **Results** toolbar, click  **Evaluation Group**.
- 2 In the **Settings** window for **Evaluation Group**, type Temperature Operating Window in the **Label** text field.
- 3 Locate the **Data** section. From the **Volume selection** list, choose **Last**.

Global Evaluation 1

- 1 Right-click **Temperature Operating Window** and choose **Global Evaluation**.
- 2 In the **Settings** window for **Global Evaluation**, locate the **Expressions** section.

3 Click  **Clear Table**.

4 In the table, enter the following settings:

Expression	Unit	Description
X_NOx_SCR	1	NOx Conversion in SCR

5 In the **Temperature Operating Window** toolbar, click  **Evaluate**.

TEMPERATURE OPERATING WINDOW



- 1 Go to the **Temperature Operating Window** window.
- 2 Click the **Table Graph** button in the window toolbar.

RESULTS

Table Graph 1

- 1 In the **Settings** window for **Table Graph**, locate the **Data** section.
- 2 From the **Plot columns** list, choose **Manual**.
- 3 In the **Columns** list box, select **NOx Conversion in SCR (1)**.
- 4 Locate the **Coloring and Style** section. From the **Width** list, choose **2**.

Temperature Operating Window

- 1 In the **Model Builder** window, under **Results** click **ID Plot Group 3**.
- 2 In the **Settings** window for **ID Plot Group**, type **Temperature Operating Window** in the **Label** text field.
- 3 Click the  **Zoom Extents** button in the **Graphics** toolbar.
- 4 In the **Temperature Operating Window** toolbar, click  **Plot**.

For convenience, add the plot groups to a **Group** with a descriptive name.

Conversion Along Reactor Axis, Temperature Increase Along Reactor Axis, Temperature Operating Window



- 1 In the **Model Builder** window, under **Results**, Ctrl-click to select **Conversion Along Reactor Axis**, **Temperature Increase Along Reactor Axis**, and **Temperature Operating Window**.
- 2 Right-click and choose **Group**.

SCR Temperature Operating Window, ANR = 1.3, Case 2

In the **Settings** window for **Group**, type **SCR Temperature Operating Window, ANR = 1.3, Case 2** in the **Label** text field.

Figure 1, Figure 2, and Figure 3 are now done. Continue by investigating the SCR operation as a function of both inlet temperature and ammonia to NO_x ratio (ANR). Such a study will generate a lot of data due to the many parameter combinations. Therefore, turn off generate default plots, choose **Only plot when requested**, and limit the data stored.

ADD STUDY

- 1 In the **Study** 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 **Preset Studies for Selected Physics Interfaces > Stationary Plug Flow**.
- 4 Click the **Add Study** button in the window toolbar.
- 5 In the **Study** toolbar, click  **Add Study** to close the **Add Study** window.

STUDY 2

Step 1: Stationary Plug Flow

In the **Model Builder** window, under **Study 2** right-click **Step 1: Stationary Plug Flow** and choose **Delete**.

STUDY 1: SCR TEMPERATURE OPERATING WINDOW, ANR = 1.3, CASE 2

In the **Model Builder** window, under **Study 1: SCR Temperature Operating Window, ANR = 1.3, Case 2** right-click **Step 1: Stationary Plug Flow** and choose **Copy**.

STUDY 2: SCR TEMPERATURE OPERATING WINDOW, ANR EFFECT, CASE 2

In the **Model Builder** window, right-click **Study 2** and choose **Paste Stationary Plug Flow**.


- 1 In the **Settings** window for **Stationary Plug Flow**, locate the **Study Extensions** section.
- 2 Click **+ Add**.
- 3 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
ANR (Ammonia to NO _x ratio in gas entering the reactor)	range(1,0.1,1.6)	

- 4 From the **Sweep type** list, choose **All combinations**.
- 5 Locate the **Study Settings** section. In the **Output volumes** text field, type range(0, V_SCR/10, V_SCR).
- 6 In the **Model Builder** window, click **Study 2**.

- 7 In the **Settings** window for **Study**, locate the **Study Settings** section.
- 8 Clear the **Generate default plots** checkbox.
- 9 In the **Label** text field, type **Study 2: SCR Temperature Operating Window, ANR Effect, Case 2**.


Solution 2 (sol2)

- 1 In the **Study** toolbar, click  **Show Default Solver**.
- 2 In the **Model Builder** window, expand the **Solution 2 (sol2)** node, then click **Dependent Variables 1**.
- 3 In the **Settings** window for **Dependent Variables**, locate the **Scaling** section.
- 4 From the **Method** list, choose **Initial-value based**.
- 5 In the **Model Builder** window, under **Study 2: SCR Temperature Operating Window, ANR Effect, Case 2 > Solver Configurations > Solution 2 (sol2)** click **Plug Flow Solver 1**.
- 6 In the **Settings** window for **Plug Flow Solver**, locate the **General** section.
- 7 From the **Volumes to store** list, choose **Output volumes by interpolation**.

RESULTS

- 1 In the **Model Builder** window, click **Results**.
- 2 In the **Settings** window for **Results**, locate the **Update of Results** section.
- 3 Select the **Only plot when requested** checkbox.

STUDY 2: SCR TEMPERATURE OPERATING WINDOW, ANR EFFECT, CASE 2

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

The following steps generate [Figure 4](#).

RESULTS

Temperature Operating Window and ANR Effect, NO_x Conversion

- 1 In the **Model Builder** window, right-click **Temperature Operating Window** and choose **Duplicate**.
- 2 In the **Settings** window for **Evaluation Group**, type **Temperature Operating Window and ANR Effect, NO_x Conversion** in the **Label** text field.
- 3 Locate the **Data** section. From the **Dataset** list, choose **None**.

Global Evaluation 1

- 1 In the **Model Builder** window, expand the **Temperature Operating Window and ANR Effect, NO_x Conversion** node, then click **Global Evaluation 1**.

- 2 In the **Settings** window for **Global Evaluation**, locate the **Data** section.
- 3 From the **Dataset** list, choose **Study 2: SCR Temperature Operating Window, ANR Effect, Case 2/Solution 2 (sol2)**.
- 4 From the **Parameter selection (ANR)** list, choose **From list**.
- 5 In the **Parameter values (ANR)** list box, select **1**.
- 6 From the **Volume selection** list, choose **Last**.
- 7 From the **Table columns** list, choose **ANR**.

Global Evaluation 2

- 1 Right-click **Results > Temperature Operating Window and ANR Effect, NOx Conversion > Global Evaluation 1** and choose **Duplicate**.
- 2 In the **Settings** window for **Global Evaluation**, locate the **Data** section.
- 3 In the **Parameter values (ANR)** list box, select **1.1**.

Global Evaluation 3

- 1 Right-click **Global Evaluation 2** and choose **Duplicate**.
- 2 In the **Settings** window for **Global Evaluation**, locate the **Data** section.
- 3 In the **Parameter values (ANR)** list box, select **1.2**.

Global Evaluation 4

- 1 Right-click **Global Evaluation 3** and choose **Duplicate**.
- 2 In the **Settings** window for **Global Evaluation**, locate the **Data** section.
- 3 In the **Parameter values (ANR)** list box, select **1.3**.

Global Evaluation 5

- 1 Right-click **Global Evaluation 4** and choose **Duplicate**.
- 2 In the **Settings** window for **Global Evaluation**, locate the **Data** section.
- 3 In the **Parameter values (ANR)** list box, select **1.4**.

Global Evaluation 6


- 1 Right-click **Global Evaluation 5** and choose **Duplicate**.
- 2 In the **Settings** window for **Global Evaluation**, locate the **Data** section.
- 3 In the **Parameter values (ANR)** list box, select **1.5**.

Global Evaluation 7

- 1 Right-click **Global Evaluation 6** and choose **Duplicate**.
- 2 In the **Settings** window for **Global Evaluation**, locate the **Data** section.

- 3 In the **Parameter values (ANR)** list box, select **1.6**.

Temperature Operating Window and ANR Effect, NO_x Conversion

- 1 In the **Model Builder** window, click **Temperature Operating Window and ANR Effect, NO_x Conversion**.
- 2 In the **Temperature Operating Window and ANR Effect, NO_x Conversion** toolbar, click  **Evaluate**.

TEMPERATURE OPERATING WINDOW AND ANR EFFECT, NO_x CONVERSION

- 1 Go to the **Temperature Operating Window and ANR Effect, NO_x Conversion** window.
- 2 Click the **Table Graph** button in the window toolbar.

RESULTS

ANR = 1.0

- 1 In the **Settings** window for **Table Graph**, type ANR = 1.0 in the **Label** text field.
- 2 Locate the **Data** section. From the **Plot columns** list, choose **Manual**.
- 3 In the **Columns** list box, select **ANR=1, NO_x Conversion in SCR (1)**.
- 4 Locate the **Coloring and Style** section. From the **Width** list, choose **2**.
- 5 Click to expand the **Legends** section. Select the **Show legends** checkbox.
- 6 Find the **Include** subsection. Select the **Label** checkbox.
- 7 Clear the **Headers** checkbox.

ANR = 1.1

- 1 Right-click **ANR = 1.0** and choose **Duplicate**.
- 2 In the **Settings** window for **Table Graph**, type ANR = 1.1 in the **Label** text field.
- 3 Locate the **Data** section. In the **Columns** list box, select **ANR=1.1, NO_x Conversion in SCR (1)**.

ANR = 1.2

- 1 Right-click **ANR = 1.1** and choose **Duplicate**.
- 2 In the **Settings** window for **Table Graph**, type ANR = 1.2 in the **Label** text field.
- 3 Locate the **Data** section. In the **Columns** list box, select **ANR=1.2, NO_x Conversion in SCR (1)**.

ANR = 1.3

- 1 Right-click **ANR = 1.2** and choose **Duplicate**.
- 2 In the **Settings** window for **Table Graph**, type ANR = 1.3 in the **Label** text field.

- 3 Locate the **Data** section. In the **Columns** list box, select **ANR=1.3, NOx Conversion in SCR (1)**.

ANR = 1.4

- 1 Right-click **ANR = 1.3** and choose **Duplicate**.
- 2 In the **Settings** window for **Table Graph**, type **ANR = 1.4** in the **Label** text field.
- 3 Locate the **Data** section. In the **Columns** list box, select **ANR=1.4, NOx Conversion in SCR (1)**.



ANR = 1.5

- 1 Right-click **ANR = 1.4** and choose **Duplicate**.
- 2 In the **Settings** window for **Table Graph**, type **ANR = 1.5** in the **Label** text field.
- 3 Locate the **Data** section. In the **Columns** list box, select **ANR=1.5, NOx Conversion in SCR (1)**.

ANR = 1.6

- 1 Right-click **ANR = 1.5** and choose **Duplicate**.
- 2 In the **Settings** window for **Table Graph**, type **ANR = 1.6** in the **Label** text field.
- 3 Locate the **Data** section. In the **Columns** list box, select **ANR=1.6, NOx Conversion in SCR (1)**.

NOx Conversion in SCR

- 1 In the **Model Builder** window, under **Results** click **ID Plot Group 4**.
- 2 In the **Settings** window for **ID Plot Group**, type **NOx Conversion in SCR** in the **Label** text field.
- 3 Locate the **Plot Settings** section.
- 4 Select the **y-axis label** checkbox. In the associated text field, type **NOx Conversion in SCR (1)**.
- 5 Locate the **Legend** section. From the **Position** list, choose **Lower middle**.
- 6 Click the  **Zoom Extents** button in the **Graphics** toolbar.
- 7 In the **NOx Conversion in SCR** toolbar, click  **Plot**.

The following steps generate [Figure 5](#).

Temperature Operating Window and ANR Effect, NH3 Conversion

- 1 In the **Model Builder** window, right-click **Temperature Operating Window and ANR Effect, NOx Conversion** and choose **Duplicate**.

- 2 In the **Model Builder** window, click **Temperature Operating Window and ANR Effect, NOx Conversion 1**.
- 3 In the **Settings** window for **Evaluation Group**, type Temperature Operating Window and ANR Effect, NH3 Conversion in the **Label** text field.

Global Evaluation 1

- 1 In the **Model Builder** window, click **Global Evaluation 1**.
- 2 In the **Settings** window for **Global Evaluation**, locate the **Expressions** section.
- 3 In the table, enter the following settings:

Expression	Unit	Description
X_NH3_SCR	1	NH3 Conversion in SCR

Global Evaluation 2

- 1 In the **Model Builder** window, click **Global Evaluation 2**.
- 2 In the **Settings** window for **Global Evaluation**, locate the **Expressions** section.
- 3 In the table, enter the following settings:

Expression	Unit	Description
X_NH3_SCR	1	NH3 Conversion in SCR

Global Evaluation 3

- 1 In the **Model Builder** window, click **Global Evaluation 3**.
- 2 In the **Settings** window for **Global Evaluation**, locate the **Expressions** section.
- 3 In the table, enter the following settings:

Expression	Unit	Description
X_NH3_SCR	1	NH3 Conversion in SCR

Global Evaluation 4

- 1 In the **Model Builder** window, click **Global Evaluation 4**.
- 2 In the **Settings** window for **Global Evaluation**, locate the **Expressions** section.
- 3 In the table, enter the following settings:

Expression	Unit	Description
X_NH3_SCR	1	NH3 Conversion in SCR

Global Evaluation 5

- 1 In the **Model Builder** window, click **Global Evaluation 5**.

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

3 In the table, enter the following settings:

Expression	Unit	Description
X_NH3_SCR	1	NH3 Conversion in SCR

Global Evaluation 6

1 In the **Model Builder** window, click **Global Evaluation 6**.

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

3 In the table, enter the following settings:

Expression	Unit	Description
X_NH3_SCR	1	NH3 Conversion in SCR

Global Evaluation 7

1 In the **Model Builder** window, click **Global Evaluation 7**.


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

3 In the table, enter the following settings:

Expression	Unit	Description
X_NH3_SCR	1	NH3 Conversion in SCR

Temperature Operating Window and ANR Effect, NH3 Conversion

1 In the **Model Builder** window, click **Temperature Operating Window and ANR Effect, NH3 Conversion**.

2 In the **Temperature Operating Window and ANR Effect, NH3 Conversion** toolbar, click  **Evaluate**.

NH3 Conversion in SCR

1 In the **Model Builder** window, right-click **NOx Conversion in SCR** and choose **Duplicate**.

2 In the **Model Builder** window, click **NOx Conversion in SCR 1**.

3 In the **Settings** window for **ID Plot Group**, type NH3 Conversion in SCR in the **Label** text field.

4 Locate the **Plot Settings** section.

5 Select the **y-axis label** checkbox. In the associated text field, type NH₃ Conversion in SCR (1).

6 Locate the **Legend** section. From the **Position** list, choose **Lower right**.

ANR = 1.0

- 1 In the **Model Builder** window, click **ANR = 1.0**.
- 2 In the **Settings** window for **Table Graph**, locate the **Data** section.
- 3 From the **Evaluation group** list, choose **Temperature Operating Window and ANR Effect, NH3 Conversion**.

ANR = 1.1

- 1 In the **Model Builder** window, click **ANR = 1.1**.
- 2 In the **Settings** window for **Table Graph**, locate the **Data** section.
- 3 From the **Evaluation group** list, choose **Temperature Operating Window and ANR Effect, NH3 Conversion**.

ANR = 1.2

- 1 In the **Model Builder** window, click **ANR = 1.2**.
- 2 In the **Settings** window for **Table Graph**, locate the **Data** section.
- 3 From the **Evaluation group** list, choose **Temperature Operating Window and ANR Effect, NH3 Conversion**.

ANR = 1.3

- 1 In the **Model Builder** window, click **ANR = 1.3**.
- 2 In the **Settings** window for **Table Graph**, locate the **Data** section.
- 3 From the **Evaluation group** list, choose **Temperature Operating Window and ANR Effect, NH3 Conversion**.

ANR = 1.4



- 1 In the **Model Builder** window, click **ANR = 1.4**.
- 2 In the **Settings** window for **Table Graph**, locate the **Data** section.
- 3 From the **Evaluation group** list, choose **Temperature Operating Window and ANR Effect, NH3 Conversion**.

ANR = 1.5

- 1 In the **Model Builder** window, click **ANR = 1.5**.
- 2 In the **Settings** window for **Table Graph**, locate the **Data** section.
- 3 From the **Evaluation group** list, choose **Temperature Operating Window and ANR Effect, NH3 Conversion**.

ANR = 1.6

- 1 In the **Model Builder** window, click **ANR = 1.6**.

- 2 In the **Settings** window for **Table Graph**, locate the **Data** section.
- 3 From the **Evaluation group** list, choose **Temperature Operating Window and ANR Effect, NH3 Conversion**.
- 4 Click the  **Zoom Extents** button in the **Graphics** toolbar.
- 5 In the **NH3 Conversion in SCR** toolbar, click  **Plot**.

NH3 Conversion in SCR, NOx Conversion in SCR

- 1 In the **Model Builder** window, under **Results**, Ctrl-click to select **NOx Conversion in SCR** and **NH3 Conversion in SCR**.
- 2 Right-click and choose **Group**.



SCR Temperature Operating Window and ANR Effect, Case 2

- 1 In the **Settings** window for **Group**, type SCR Temperature Operating Window and ANR Effect, Case 2 in the **Label** text field.

We have now investigated the influence of both inlet temperature and ammonia to NOx ratio on the SCR monolith system. Now solve for both of the catalysts in series. Begin by turning off the functionality to only plot when requested.

- 2 In the **Model Builder** window, click **Results**.
- 3 In the **Settings** window for **Results**, locate the **Update of Results** section.
- 4 Clear the **Only plot when requested** checkbox.

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 **Preset Studies for Selected Physics Interfaces > Stationary Plug Flow**.
- 4 Click the **Add Study** button in the window toolbar.
- 5 In the **Home** toolbar, click  **Add Study** to close the **Add Study** window.

STUDY 3

Stationary Plug Flow, SCR

- 1 In the **Settings** window for **Stationary Plug Flow**, type Stationary Plug Flow, SCR in the **Label** text field.
- 2 Locate the **Study Settings** section. In the **Output volumes** text field, type 0 V_SCR.
- 3 Locate the **Physics and Variables Selection** section. In the **Solve for** column of the table, under **Component 1 (comp1)**, clear the checkbox for **Ammonia Slip Catalyst (ASC) (re2)**.

Stationary Plug Flow, ASC

- 1 Right-click **Study 3** > **Step 1: Stationary Plug Flow, SCR** and choose **Duplicate**.
- 2 In the **Settings** window for **Stationary Plug Flow**, type Stationary Plug Flow, ASC in the **Label** text field.
- 3 Locate the **Study Settings** section. In the **Output volumes** text field, type V_SCR $V_SCR + V_ASC$.
- 4 Locate the **Physics and Variables Selection** section. In the **Solve for** column of the table, under **Component 1 (comp1)**, select the checkbox for **Ammonia Slip Catalyst (ASC) (re2)**.
- 5 In the **Solve for** column of the table, under **Component 1 (comp1)**, clear the checkbox for **Selective Catalytic Reduction Catalyst (SCR) (re)**.

To connect the two beds we need to create the dataset for the study.

- 6 In the **Model Builder** window, click **Study 3**.
- 7 In the **Settings** window for **Study**, type Study 3: Single Channel Model, Influence of ANR, Case 2 in the **Label** text field.
- 8 Locate the **Study Settings** section. Select the **Store solution for all intermediate study steps** checkbox.
- 9 Clear the **Generate default plots** checkbox.
- 10 In the **Study** toolbar, click $t=0$ **Get Initial Value**.

We can now connect the two **Reaction Engineering** interfaces with each other, so that the second catalyst uses the output from the first catalyst as input.

- 11 In the **Model Builder** window, click **Step 2: Stationary Plug Flow, ASC**.
- 12 In the **Settings** window for **Stationary Plug Flow**, click to expand the **Values of Dependent Variables** section.
- 13 Find the **Initial values of variables solved for** subsection. From the **Settings** list, choose **User controlled**.
- 14 From the **Method** list, choose **Initial expression**.
- 15 From the **Selection** list, choose **Last**.
- 16 Find the **Values of variables not solved for** subsection. From the **Settings** list, choose **User controlled**.
- 17 From the **Selection** list, choose **Last**.

Use initial value based scales for the dependent variables.

Solver Configurations


In the **Model Builder** window, expand the **Study 3: Single Channel Model, Influence of ANR, Case 2 > Solver Configurations** node.

Solution 3 (sol3)

- 1 In the **Model Builder** window, expand the **Study 3: Single Channel Model, Influence of ANR, Case 2 > Solver Configurations > Solution 3 (sol3)** node, then click **Dependent Variables 1**.
- 2 In the **Settings** window for **Dependent Variables**, locate the **Scaling** section.
- 3 From the **Method** list, choose **Initial-value based**.
- 4 In the **Model Builder** window, click **Dependent Variables 2**.
- 5 In the **Settings** window for **Dependent Variables**, locate the **Scaling** section.
- 6 From the **Method** list, choose **Initial-value based**.

Add a **Parametric Sweep** feature to solve for three different ammonia to NO_x ratios.

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 In the table, enter the following settings:


Parameter name	Parameter value list	Parameter unit
ANR (Ammonia to NO _x ratio in gas entering the reactor)	1 1.3 1.6	

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

The following steps generate [Figure 6](#).


RESULTS

Molar Fraction of NH₃ and NO_x

- 1 In the **Results** toolbar, click  **ID Plot Group**.
- 2 In the **Settings** window for **ID Plot Group**, type Molar Fraction of NH₃ and NO_x in the **Label** text field.
- 3 Locate the **Data** section. From the **Dataset** list, choose **Study 3: Single Channel Model, Influence of ANR, Case 2/Parametric Solutions 2 (sol6)**.

NH₃ SCR

- 1 Right-click **Molar Fraction of NH₃ and NO_x** and choose **Global**.

- 2 In the **Settings** window for **Global**, type NH3 SCR in the **Label** text field.
- 3 Locate the **y-Axis Data** section. Click  **Clear Table**.
- 4 Click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1) > Definitions > Variables > yNH3_SCR - Molar fraction of NH3 in SCR catalytic bed - 1**.
- 5 Locate the **y-Axis Data** section. In the table, enter the following settings:

Expression	Unit	Description
yNH3_SCR	ppm	Molar fraction of NH3 in SCR catalytic bed

- 6 Locate the **Coloring and Style** section. Find the **Line style** subsection. From the **Line** list, choose **Cycle**.
- 7 From the **Color** list, choose **Blue**.
- 8 From the **Width** list, choose **2**.
- 9 Locate the **Legends** section. Clear the **Show legends** checkbox.

NH3

- 1 Right-click **NH3 SCR** and choose **Duplicate**.
- 2 In the **Settings** window for **Global**, type NH3 in the **Label** text field.
- 3 Locate the **Data** section. From the **Dataset** list, choose **Study 3: Single Channel Model, Influence of ANR, Case 2/Parametric Solutions 1 (sol5)**.
- 4 Locate the **y-Axis Data** section. In the table, enter the following settings:

Expression	Unit	Description
yNH3_ASC	ppm	Molar fraction of NH3 in ASC

- 5 Locate the **Coloring and Style** section. Find the **Line style** subsection. From the **Line** list, choose **Cycle (reset)**.
- 6 Locate the **Legends** section. Select the **Show legends** checkbox.
- 7 Find the **Include** subsection. Clear the **Expression** checkbox.
- 8 Find the **Prefix and suffix** subsection. In the **Prefix** text field, type NH_3 .

NO_x SCR

- 1 In the **Model Builder** window, right-click **NH3 SCR** and choose **Duplicate**.
- 2 In the **Settings** window for **Global**, type NO_x SCR in the **Label** text field.

3 Locate the **y-Axis Data** section. In the table, enter the following settings:

Expression	Unit	Description
yNOx_SCR	ppm	Molar fraction of NOx in SCR catalytic bed

4 Locate the **Coloring and Style** section. Find the **Line style** subsection. From the **Line** list, choose **Cycle (reset)**.

5 From the **Color** list, choose **Magenta**.

NO_x

1 Right-click **NO_x SCR** and choose **Duplicate**.

2 In the **Settings** window for **Global**, type NO_x in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Study 3: Single Channel Model, Influence of ANR, Case 2/Parametric Solutions I (sol5)**.

4 Locate the **y-Axis Data** section. In the table, enter the following settings:

Expression	Unit	Description
yNOx_ASC	ppm	Molar fraction of NOx in ASC

5 Locate the **Legends** section. Select the **Show legends** checkbox.

6 Find the **Include** subsection. Select the **Label** checkbox.

7 Clear the **Expression** checkbox.

Molar Fraction of NH₃ and NO_x

1 In the **Model Builder** window, click **Molar Fraction of NH₃ and NO_x**.

2 In the **Settings** window for **ID Plot Group**, locate the **Title** section.

3 From the **Title type** list, choose **None**.

4 Locate the **Plot Settings** section.

5 Select the **x-axis label** checkbox. In the associated text field, type Reactor volume (m³).


6 Select the **y-axis label** checkbox. In the associated text field, type Molar Fraction of NH₃ (ppm).

7 Select the **Two y-axes** checkbox.

8 In the table, enter the following settings:

Plot	Plot on secondary y-axis
NH3 SCR	
NH3	
NOx SCR	√
NOx	√

9 Select the **Secondary y-axis label** checkbox. In the associated text field, type Molar Fraction of NOx (ppm).

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

11 In the **Molar Fraction of NH3 and NOx** toolbar, click  **Plot**.

The following steps generate [Figure 7](#).

Conversion of NH3 and NOx

1 Right-click **Molar Fraction of NH3 and NOx** and choose **Duplicate**.

2 In the **Model Builder** window, click **Molar Fraction of NH3 and NOx I**.

3 In the **Settings** window for **ID Plot Group**, type Conversion of NH3 and NOx in the **Label** text field.

4 Locate the **Plot Settings** section. In the **y-axis label** text field, type Conversion (1).

5 Clear the **Two y-axes** checkbox.

6 Locate the **Legend** section. From the **Position** list, choose **Lower right**.

NH3 SCR

1 In the **Model Builder** window, click **NH3 SCR**.

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 (comp I) > Definitions > Variables > X_NH3_SCR - NH3 Conversion in SCR - I**.

3 Locate the **y-Axis Data** section. In the table, enter the following settings:

Expression	Unit	Description
X_NH3_SCR	1	NH3 Conversion in SCR

NH3

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

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

3 In the table, enter the following settings:

Expression	Unit	Description
X_NH3_tot	1	NH3 Conversion in SCR

NO_x SCR



- 1 In the **Model Builder** window, click **NO_x SCR**.
- 2 In the **Settings** window for **Global**, locate the **y-Axis Data** section.
- 3 In the table, enter the following settings:

Expression	Unit	Description
X_NOx_SCR	1	NOx Conversion in SCR

NO_x

- 1 In the **Model Builder** window, click **NO_x**.
- 2 In the **Settings** window for **Global**, locate the **y-Axis Data** section.
- 3 In the table, enter the following settings:

Expression	Unit	Description
X_NOx_tot	1	Total NOx Conversion in System (SCR + ASC)

- 4 Click the  **Zoom Extents** button in the **Graphics** toolbar.
- 5 In the **Conversion of NH₃ and NO_x** toolbar, click  **Plot**.

The intermediate engine load case, referred to as case 2, has now been investigated, both in terms of temperature and ANR. How well does the system perform for other engine loads? Add a final study to investigate three different load cases for an ANR = 1.3.

Conversion of NH₃ and NO_x, Molar Fraction of NH₃ and NO_x


- 1 In the **Model Builder** window, under **Results**, Ctrl-click to select **Molar Fraction of NH₃ and NO_x** and **Conversion of NH₃ and NO_x**.
- 2 Right-click and choose **Group**.

Single Channel Model, Influence of ANR, Case 2

In the **Settings** window for **Group**, type Single Channel Model, Influence of ANR, Case 2 in the **Label** text field.

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 **Preset Studies for Selected Physics Interfaces > Stationary Plug Flow**.
- 4 Click the **Add Study** button in the window toolbar.
- 5 In the **Home** toolbar, click  **Add Study** to close the **Add Study** window.

STUDY 4

Step 1: Stationary Plug Flow

In the **Model Builder** window, under **Study 4** right-click **Step 1: Stationary Plug Flow** and choose **Delete**.

STUDY 3: SINGLE CHANNEL MODEL, INFLUENCE OF ANR, CASE 2


Parametric Sweep, Step 1: Stationary Plug Flow, SCR, Step 2: Stationary Plug Flow, ASC

- 1 In the **Model Builder** window, under **Study 3: Single Channel Model, Influence of ANR, Case 2**, Ctrl-click to select **Parametric Sweep, Step 1: Stationary Plug Flow, SCR**, and **Step 2: Stationary Plug Flow, ASC**.
- 2 Right-click and choose **Copy**.

STUDY 4: SINGLE CHANNEL MODEL, ANR = 1.3, ALL CASES

- 1 In the **Model Builder** window, right-click **Study 4** and choose **Paste Multiple Items**.
- 2 In the **Settings** window for **Study**, type Study 4: Single Channel Model, ANR = 1.3, All Cases in the **Label** text field.
- 3 Locate the **Study Settings** section. Select the **Store solution for all intermediate study steps** checkbox.
- 4 Clear the **Generate default plots** checkbox.


Parametric Sweep

- 1 In the **Model Builder** window, under **Study 4: Single Channel Model, ANR = 1.3, All Cases** click **Parametric Sweep**.
- 2 In the **Settings** window for **Parametric Sweep**, locate the **Study Settings** section.
- 3 From the **Sweep type** list, choose **Parameter switch**.
- 4 Click  **Add**.
- 5 In the table, enter the following settings:


Switch	Cases	Case numbers
Cases	All	range(1,1,3)

Use initial value based scales for the dependent variables.

Solution 13 (sol13)

- 1 In the **Study** toolbar, click  **Show Default Solver**.
- 2 In the **Model Builder** window, expand the **Solution 13 (sol13)** node, then click **Dependent Variables 1**.
- 3 In the **Settings** window for **Dependent Variables**, locate the **Scaling** section.
- 4 From the **Method** list, choose **Initial-value based**.
- 5 In the **Model Builder** window, under **Study 4: Single Channel Model, ANR = 1.3, All Cases > Solver Configurations > Solution 13 (sol13)** click **Dependent Variables 2**.
- 6 In the **Settings** window for **Dependent Variables**, locate the **Scaling** section.
- 7 From the **Method** list, choose **Initial-value based**.

Step 2: Stationary Plug Flow, ASC

- 1 In the **Model Builder** window, under **Study 4: Single Channel Model, ANR = 1.3, All Cases** click **Step 2: Stationary Plug Flow, ASC**.
- 2 In the **Settings** window for **Stationary Plug Flow**, locate the **Values of Dependent Variables** section.
- 3 Find the **Initial values of variables solved for** subsection. From the **Study** list, choose **Study 4: Single Channel Model, ANR = 1.3, All Cases, Stationary Plug Flow, SCR**.
- 4 From the **Use** list, choose **Solution Store 2 (sol14)**.
- 5 Find the **Values of variables not solved for** subsection. From the **Study** list, choose **Study 4: Single Channel Model, ANR = 1.3, All Cases, Stationary Plug Flow, SCR**.
- 6 From the **Use** list, choose **Solution Store 2 (sol14)**.
- 7 In the **Study** toolbar, click  **Compute**.

The following steps generate [Figure 8](#) and [Figure 9](#).

RESULTS

Single Channel Model, ANR = 1.3, All Cases

- 1 In the **Model Builder** window, right-click **Single Channel Model, Influence of ANR, Case 2** and choose **Duplicate**.
- 2 In the **Settings** window for **Group**, type Single Channel Model, ANR = 1.3, All Cases in the **Label** text field.



Molar Fraction of NH₃ and NO_x, All Cases

- 1 In the **Model Builder** window, expand the **Single Channel Model, ANR = 1.3, All Cases** node, then click **Molar Fraction of NH₃ and NO_x 1**.
- 2 In the **Settings** window for **ID Plot Group**, type Molar Fraction of NH₃ and NO_x, All Cases in the **Label** text field.
- 3 Locate the **Data** section. From the **Dataset** list, choose **Study 4: Single Channel Model, ANR = 1.3, All Cases/Parametric Solutions 4 (sol16)**.

NH₃

- 1 In the **Model Builder** window, expand the **Molar Fraction of NH₃ and NO_x, All Cases** node, then click **NH₃**.
- 2 In the **Settings** window for **Global**, locate the **Data** section.
- 3 From the **Dataset** list, choose **Study 4: Single Channel Model, ANR = 1.3, All Cases/Parametric Solutions 3 (sol15)**.

NO_x

- 1 In the **Model Builder** window, click **NO_x**.
- 2 In the **Settings** window for **Global**, locate the **Data** section.
- 3 From the **Dataset** list, choose **Study 4: Single Channel Model, ANR = 1.3, All Cases/Parametric Solutions 3 (sol15)**.
- 4 Click the  **Zoom Extents** button in the **Graphics** toolbar.
- 5 In the **Molar Fraction of NH₃ and NO_x, All Cases** toolbar, click  **Plot**.



Conversion of NH₃ and NO_x, All Cases

- 1 In the **Model Builder** window, under **Results > Single Channel Model, ANR = 1.3, All Cases** click **Conversion of NH₃ and NO_x 1**.
- 2 In the **Settings** window for **ID Plot Group**, type Conversion of NH₃ and NO_x, All Cases in the **Label** text field.
- 3 Locate the **Data** section. From the **Dataset** list, choose **Study 4: Single Channel Model, ANR = 1.3, All Cases/Parametric Solutions 4 (sol16)**.

NH₃

- 1 In the **Model Builder** window, expand the **Conversion of NH₃ and NO_x, All Cases** node, then click **NH₃**.
- 2 In the **Settings** window for **Global**, locate the **Data** section.
- 3 From the **Dataset** list, choose **Study 4: Single Channel Model, ANR = 1.3, All Cases/Parametric Solutions 3 (sol15)**.

NO_x

- 1 In the **Model Builder** window, click **NO_x**.
- 2 In the **Settings** window for **Global**, locate the **Data** section.
- 3 From the **Dataset** list, choose **Study 4: Single Channel Model, ANR = 1.3, All Cases/ Parametric Solutions 3 (sol15)**.
- 4 Click the  **Zoom Extents** button in the **Graphics** toolbar.
- 5 In the **Conversion of NH₃ and NO_x, All Cases** toolbar, click  **Plot**.

The following steps generate [Figure 10](#).

Temperature Increase Along Reactor Axis, All Cases

- 1 In the **Model Builder** window, right-click **Conversion of NH₃ and NO_x, All Cases** and choose **Duplicate**.
- 2 In the **Settings** window for **ID Plot Group**, type **Temperature Increase Along Reactor Axis, All Cases** in the **Label** text field.
- 3 Locate the **Plot Settings** section. In the **y-axis label** text field, type **Temperature Increase (K)**.
- 4 In the **Model Builder** window, expand the **Temperature Increase Along Reactor Axis, All Cases** node.

NO_x, NO_x SCR

- 1 In the **Model Builder** window, under **Results > Single Channel Model, ANR = 1.3, All Cases > Temperature Increase Along Reactor Axis, All Cases**, Ctrl-click to select **NO_x SCR** and **NO_x**.
- 2 Right-click and choose **Delete**.

Temperature Increase SCR

- 1 In the **Model Builder** window, under **Results > Single Channel Model, ANR = 1.3, All Cases > Temperature Increase Along Reactor Axis, All Cases** click **NH₃ SCR**.
- 2 In the **Settings** window for **Global**, type **Temperature Increase SCR** in the **Label** text field.
- 3 Locate the **y-Axis Data** section. In the table, enter the following settings:

Expression	Unit	Description
re.T-T	K	

- 4 Locate the **Coloring and Style** section. Find the **Line style** subsection. From the **Line** list, choose **Solid**.
- 5 From the **Color** list, choose **Cycle**.

Temperature Increase ASC



- 1 In the **Model Builder** window, under **Results > Single Channel Model, ANR = 1.3, All Cases > Temperature Increase Along Reactor Axis, All Cases** click **NH3**.
- 2 In the **Settings** window for **Global**, type Temperature Increase ASC in the **Label** text field.
- 3 Locate the **y-Axis Data** section. In the table, enter the following settings:

Expression	Unit	Description
re2.T-T	K	

- 4 Locate the **Coloring and Style** section. Find the **Line style** subsection. From the **Line** list, choose **Solid**.
- 5 From the **Color** list, choose **Cycle (reset)**.
- 6 Click to expand the **Legends** section. From the **Legends** list, choose **Manual**.
- 7 In the table, enter the following settings:

Legends
Low Load
Int. Load
High Load

Temperature Increase Along Reactor Axis, All Cases

- 1 In the **Model Builder** window, click **Temperature Increase Along Reactor Axis, All Cases**.
- 2 In the **Settings** window for **ID Plot Group**, locate the **Legend** section.
- 3 In the **Number of columns** text field, type 3.
- 4 In the **Maximum relative width** text field, type 1.
- 5 Click the  **Zoom Extents** button in the **Graphics** toolbar.
- 6 In the **Temperature Increase Along Reactor Axis, All Cases** toolbar, click  **Plot**.