

INTRODUCTION TO

Chemical Reaction Engineering Module

Introduction to the Chemical Reaction Engineering Module

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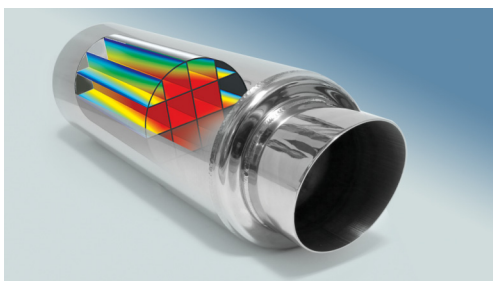
Introducing the Chemical Reaction Engineering Module

The Chemical Reaction Engineering Module is tailor-made for the modeling of chemical systems primarily affected by chemical composition, reaction kinetics, fluid flow, and temperature as functions of space and time. It has several interfaces to model chemical reaction kinetics: mass transport in dilute, concentrated, and electric potential-affected solutions; laminar and porous media flows; and energy transport.

Included in these interfaces are the kinetic expressions for reacting systems, in bulk solutions and on catalytic surfaces, and models for the definition of mass transport. You also have access to a variety of ready-made expressions in order to calculate a system's thermodynamic and transport properties.

While a major focus of the module is on chemical reactors and reacting systems, it is also extensively used for systems where mass transport is the major process. This includes unit operations equipment, separation and mixing processes, chromatography, and electrophoresis. The module is also widely used in educational and training courses to explain chemical engineering, chemical reaction engineering, electrochemical engineering, biotechnology, and transport phenomena.

In addition to its application in traditional chemical industries, it is a popular tool for investigating clean technology processes (for example, catalytic monoliths and reactive filters) for applications such as microlaboratories in biotechnology and in the development of sensors and equipment in analytical chemistry.



An overview of the interfaces and their functionality can be found in [Chemical Reaction Engineering Module Interfaces](#).

Chemical Reaction Engineering Simulations

Simulations in chemical reaction engineering are often used during the investigation and development of a reaction process or system.

In the initial stages, they are used to dissect and understand the process or system. By setting up a model and studying the results from the simulations, engineers and scientists achieve the understanding and intuition required for further innovation.

Once a process is well understood, modeling and simulations are used to optimize and control the process' variables and parameters. These “virtual” experiments are run to adapt the process to different operating conditions.

Another use for modeling is to simulate scenarios that may be difficult to investigate experimentally. One example of this is to improve safety, such as when an uncontrolled release of chemicals occurs during an accident. Simulations are used to develop protocols and procedures to prevent or contain the impact from these hypothetical accidents.

In all these cases, modeling and simulations provide value for money by reducing the need for a large number of experiments or to build prototypes, while, potentially, granting alternative and better insights into a process or design.

Modeling Strategy

The flowchart in Figure 1 describes a strategy for modeling and simulating chemical reaction processes and systems.

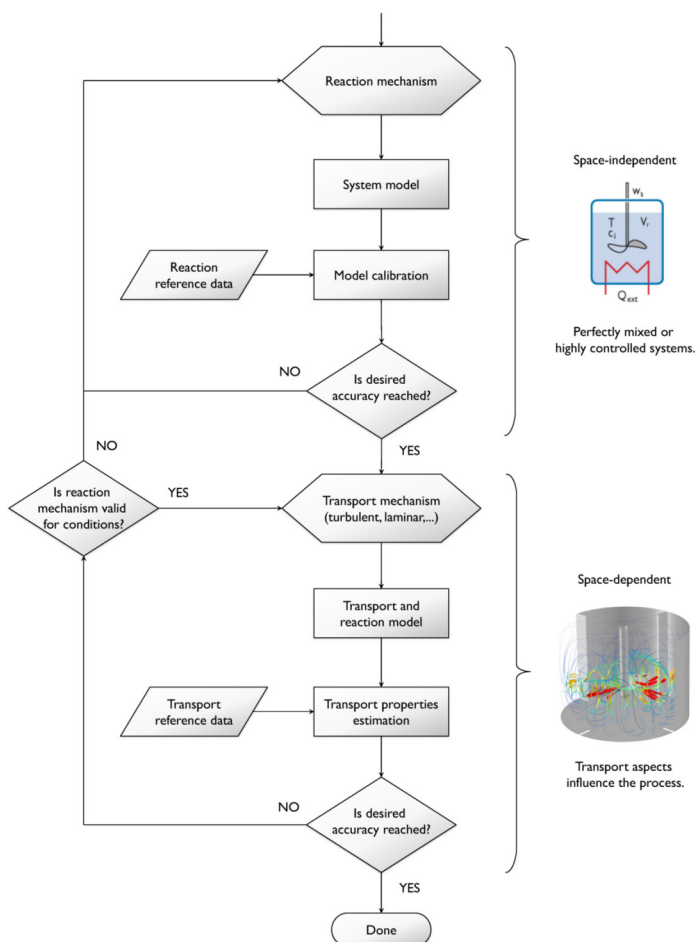


Figure 1: Flowchart summarizing the strategy for modeling reacting systems or designing chemical reactors.

The strategy suggests first investigating a reacting system that is either space-independent, or where the space dependency is very well-defined.

A system where space dependency is irrelevant is usually so well mixed that chemical species concentrations and temperature are uniform throughout and are

only a function of time — this is often denoted as a perfectly mixed reactor. A plug flow reactor is a system where the space dependency is well defined.

Once the effects of space dependency are removed or well accounted for, both experimental and modeling investigations can concentrate on the reactions themselves, and the rate laws that control them.

The next step is to apply this information to the chemical reactors or systems that are of interest. These, of course, vary in length, width, and height, and are also subject to a range of external parameters including inflows, outflows, cooling, and heating. These are space (and time) dependent systems.

Investigating Chemical Reaction Kinetics — Modeling Perfectly Mixed and Plug Flow Reactors

An important component in chemical reaction engineering is the definition of the respective reaction rate laws, which result from informed assumptions or hypotheses about the chemical reaction mechanisms. Ideally, a reaction mechanism and its corresponding rate laws are found through conducting rigidly controlled experiments, where the influence of spatial and time variations are well known. Sometimes such experiments are difficult to run, and a search of the literature or using the rate laws from similar reactions provides the first hypothesis.



Bench-scale perfectly mixed reactor.

Perfectly mixed or ideal plug flow reactor models are the most effective reactor types for duplicating and modeling the exact conditions of a rigidly-controlled experimental study. These virtual experiments are used to study the influence of various kinetic parameters and other conditions on the behavior of the reacting system. Then, using parameter estimation, the reaction rate constants for the proposed reaction mechanisms can be found by comparing experimental and simulated results. The comparison of these results to other experimental studies enables the verification or further calibration of the proposed mechanism and its kinetic parameters.

Modeling a reaction system in a well-defined reactor environment also provides an understanding of the influence of various, yet specific, operating conditions on the process, such as temperature or pressure variations. The more knowledge that is gained about a reacting system or process, the easier it is to model and simulate more advanced descriptions of these systems and processes.

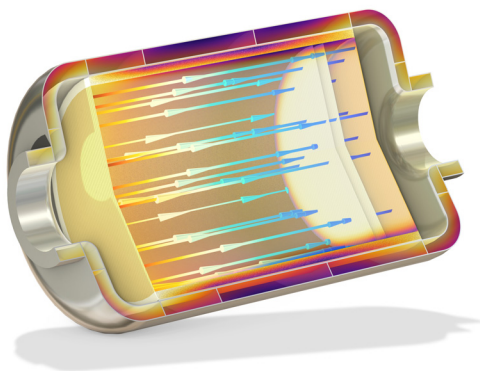
Investigating Reactors and Systems — Modeling Space Dependency

Once a reacting process or system's mechanism and kinetic parameters are decided and fine-tuned, they can be used in more advanced studies of the system or process in real-world environments. Such studies invariably require full descriptions of the variations through both time and space to be considered, which, apart from the reaction kinetics, includes material transport, heat transfer, and fluid flow.



Real world environment.

Depending on assumptions that can (or sometimes must) be made, these descriptions are done in either 1D, 2D, or 3D, where time dependency can also be considered if it is of importance.



The temperature throughout a monolith reactor with two catalytic beds. The surface plot shows the temperature that varies both radially and axially, and the arrows show the ammonia concentration, varying from high (red) to low (blue).

Once again, comparisons between simulation and results, from either the reactor or system itself, or a prototype of them, should always be done if possible. Models that involve material transport, heat transfer, and fluid flow often involve generic

material parameters that are taken from the literature or from systems that may be slightly different, and these may need to be calibrated to improve the accuracy of the model.

When a model's accuracy has been ascertained, then it becomes a model that can be used to simulate the real-world chemical reactor or process under a variety of different operating conditions. The understanding that results from these models, as well as the concrete results they provide, go toward developing or optimizing a chemical reactor with greater precision, or controlling a system with more confidence.

Chemical Reaction Engineering Module Interfaces

Figure 2 shows the physics interfaces available to model chemical species transport, fluid flow, and heat transfer when licensed to the Chemical Reaction Engineering Module. For the full list of interfaces available see also [The Physics Interface List by Space Dimension and Study Type](#).

- ▼  Chemical Species Transport
 -  Transport of Diluted Species (tds)
 -  Transport of Concentrated Species (tcs)
 -  Chemistry (chem)
 -  Development Flowsheet (fs)
 -  Reaction Engineering (re)
 -  Nernst-Planck Equations (npe)
 -  Nernst-Planck-Poisson Equations
 -  Electrophoretic Transport (el)
 -  Transport of Diluted Species in Porous Media (tds)
 -  Transport of Concentrated Species in Porous Media (tcs)
- ▼  Reacting Flow
 -  Laminar Flow, Diluted Species
 -  Laminar Flow, Concentrated Species
- ▼  Reacting Flow in Porous Media
 -  Transport of Diluted Species
 -  Transport of Concentrated Species
 - >  Porous Catalyst
 - >  Packed Bed
 - >  Moving Bed
- ▼  Nonisothermal Reacting Flow
 - >  Porous Media Flow
 -  Laminar Flow
- ▼  Dispersed Two-Phase Flow with Species Transport
 -  Laminar Flow
- ▼  Vapor-Liquid Equilibrium
 -  Laminar Vapor Flow
 -  Laminar Two-Phase Flow
- ▼  Precipitation and Crystallization
 -  Size-Based Population Balance (pbsb)
 -  Precipitation and Crystallization in Fluid Flow
 -  Surface Reactions (sr)
 -  Transport of Diluted Species in Fractures (dsf)
- ▼  Fluid Flow
 - ▼  Single-Phase Flow
 -  Creeping Flow (spf)
 -  Laminar Flow (spf)
 - ▼  Multiphase Flow
 - >  Mixture Model
 - ▼  Porous Media and Subsurface Flow
 -  Brinkman Equations (br)
 -  Darcy's Law (dl)
 -  Free and Porous Media Flow, Brinkman (fp)
 -  Free and Porous Media Flow, Darcy
 - ▼  Nonisothermal Flow
 -  Laminar Flow
 -  Brinkman Equations
 - ▼  Fluid-Structure Interaction
 -  Fluid-Solid Interaction, Fixed Geometry
- ▼  Heat Transfer
 -  Heat Transfer in Solids (ht)
 -  Heat Transfer in Fluids (ht)
 -  Heat Transfer in Solids and Fluids (ht)
 - ▼  Conjugate Heat Transfer
 -  Laminar Flow
 - ▼  Electromagnetic Heating
 -  Joule Heating
 -  Induction Heating
 - ▼  Porous Media
 -  Heat Transfer in Porous Media (ht)
 -  Heat Transfer in Packed Beds (ht)

Figure 2: The physics interface list for the Chemical Reaction Engineering Module as shown in the Model Wizard for a 3D model (left: interfaces under the Chemical Species Transport branch; right interfaces under the Fluid Flow and Heat Transfer branches).

By combining the Chemical Reaction Engineering Module with the CFD, and Heat Transfer Module, you are also able to incorporate turbulent flow, multiphase flow, and nonisothermal flow, as well as radiation heat transfer.

CHEMICAL REACTION AND MASS TRANSPORT

The Reaction Engineering interface () includes all of the tools required to simulate chemical reaction kinetics in well-defined environments. It sets up

simulations of reversible, equilibrium, and irreversible reactions in volumes or on surfaces. You can study the evolution of species concentrations and temperature in controlled environments described by batch, continuous stirred-tank, semibatch, and plug flow reactors. Using the Parameter Estimation Study, multiple objectives may be optimized, and with the Optimization Module, additional methods become available.

The Chemistry interface () provides libraries of chemical reactions for use by other physics interfaces. It also provides kinetic expressions for reaction rates, reaction heat sources, and species transport properties to other interfaces. This interface is always created when a Reaction Engineering model is exported to a space-dependent model. As such, it serves as a reaction kinetics and material property provider to the space-dependent transport interfaces, such as Transport of Diluted Species.

The Transport of Diluted Species interface () simulates transport of chemical species in a dilute solution. The concentration of one or several chemical species is solved for, and transport mechanisms such as diffusion, convection, and migration in electric fields are included. Transport and reactions of species in gaseous, liquid, and solid solutions can be modeled. This interface also supports transport in porous media such as porous catalysts and packed beds (possibly moving). Contrary to the Transport of Concentrated Species interface () , the concentrations of the species modeled are assumed to not affect the properties of the solution.

The Transport of Concentrated Species interface () models chemical species transport by diffusion, convection, and migration in mixtures where transport properties, such as diffusion, depend on the composition of the mixture. This interface supports multicomponent transport models given by Fickian diffusion, a mixture-average model, as well as the Maxwell-Stefan equations. Similar to the Transport of Diluted Species interface, it also handles transport in porous media. It supports cases where either the solid phase substrate is exclusively immobile, or when a gas-filling medium is assumed to be immobile.

The Nernst–Planck Equations interface () includes a migration term, along with convection and diffusion mass transport, together with an equation that guarantees electroneutrality. Apart from species concentrations, the interface also solves for the electric potential.

The Nernst–Planck–Poisson Equations interface () is a multiphysics interface for modeling transport of electrolyte species without the otherwise common assumption of local electroneutrality. This allows you to simulate charge separation typically arising close to an electrode surface, where electrolyte ions are attracted and repelled by unscreened excess charge on the electrode. The charge separation region, also called the diffuse double layer, normally extends a few nanometers away from the electrode surface into the electrolyte.

The Electrophoretic Transport interface () is used to solve for the transport of species in water-based system subject to potential gradients. The species transported can be any combination of weak and strong acids and bases, ampholytes, and uncharged species. The interface supports dissociation equilibria for weak acids, bases, and ampholytes, as well as the water auto-ionization reaction.

The Laminar Flow, Concentrated Species interface () under Reacting Flow combines the functionality of the Single-Phase Flow and Transport of Concentrated Species interface.

The Laminar Flow, Diluted Species interface () under Reacting Flow combines the functionality of the Single-Phase Flow interface with functionality of the Transport of Diluted Species interface.

The Reacting Flow in Porous Media, Transport of Diluted Species interface () treats diluted reacting mixtures transported by a free and/or porous media flow. This multiphysics interface combines the functionality of the Brinkman Equations and Transport of Diluted Species in Porous Media interface.

The Reacting Flow in Porous Media, Transport of Concentrated Species interface () treats concentrated reacting mixtures transported by a free and/or porous media flow. This multiphysics interface combines the functionality of the Brinkman Equations and Transport of Concentrated Species interface.

The Reacting Flow in Porous Media, Porous Catalyst, Transport of Diluted Species interface () treats diluted reacting mixtures transported by a free and/or porous media flow in a catalytic reactor. This multiphysics interface combines the functionality of the Brinkman Equations and Transport of Diluted Species in Porous Catalysts interface.

The Reacting Flow in Porous Media, Porous Catalyst, Transport of Concentrated Species interface () treats concentrated reacting mixtures transported by a free and/or porous media flow in a catalytic reactor. This multiphysics interface combines the functionality of the Brinkman Equations and Transport of Concentrated Species in Porous Catalysts interface.

The Reacting Flow in Porous Media, Packed Bed, Transport of Diluted Species interface () treats diluted reacting mixtures transported by a free and/or porous media flow in a reactive pellet bed reactor. This multiphysics interface combines the functionality of the Brinkman Equations and Transport of Diluted Species in Packed Beds.

The Reacting Flow in Porous Media, Packed Bed, Transport of Concentrated Species interface () treats concentrated reacting mixtures transported by a free and/or porous media flow in a reactive pellet bed reactor. This multiphysics interface combines the functionality of the Brinkman Equations and Transport of Concentrated Species in Packed Beds.

The Reacting Flow in Porous Media, Moving Bed, Transport of Diluted Species interface, Shrinking Core Model () treats diluted reacting mixtures transported by a free and/or porous media flow in a reactive moving pellet bed reactor where pellet acts as reactant. This multiphysics interface combines the functionality of the Brinkman Equations and Transport of Diluted Species in Packed Beds.

The Reacting Flow in Porous Media, Moving Bed, Transport of Concentrated Species interface () treats concentrated reacting mixtures transported by a free and/or porous media flow in a reactive moving pellet bed reactor. This multiphysics interface combines the functionality of the Brinkman Equations and Transport of Concentrated Species in Packed Beds.

The Reacting Flow in Porous Media, Moving Bed, Transport of Diluted Species interface, Shrinking Core Model () treats diluted reacting mixtures transported by a free and/or porous media flow in a reactive moving pellet bed reactor where pellet acts as reactant. This multiphysics interface combines the functionality of the Brinkman Equations and Transport of Diluted Species in Packed Beds.

The Nonisothermal Reacting Flow, Brinkman Equations interface () combines Chemistry, Transport of Concentrated Species in Porous Media, Brinkman Equations, and Heat Transfer in Porous Media interfaces to treat the reacting flow and reactions in porous media. The Heat Transfer in Fluids can take reaction heat and species enthalpy from Chemistry.

The Nonisothermal Reacting Flow, Laminar Flow interface () combines Chemistry, Transport of Concentrated Species, Laminar Flow and Heat Transfer in Fluids interfaces to treat reacting flow. The Heat Transfer in Fluids can take reaction heat and species enthalpy from Chemistry.

The Dispersed Two-Phase Laminar Flow with Species Transport interface () models dispersed two-phase fluid flow with mass transfer. The interface combines Mixture Model, Laminar Flow with mass transport in both the continuous phase and the dispersed phase. The interface can for example be used to model liquid-liquid extraction.

The Size-Based Population Balance interface () , under Precipitation and Crystallization, is used to model the population balance of particles in a fluid. Examples include crystals in a liquid, gas bubbles in a liquid, and droplets in a gas. The interface solves for the discretized size distribution of particles, with support for growth, nucleation, aggregation, and breakage terms.

The Precipitation and Crystallization interface () , under Precipitation and Crystallization, is available in 0D. It is used to simulate precipitation of chemical species in a solution and to solve for the resulting size distribution of the precipitate. It couples the Reaction Engineering and Size-Based Population Balance interfaces.

The Precipitation and Crystallization in Fluid Flow interface () , under Precipitation and Crystallization, is used to simulate precipitation of chemical species in a solution and to solve for the resulting size distribution of the precipitate. It combines the Laminar Flow, Transport of Diluted Species and Size-Based Population Balance interfaces.

The Laminar Vapor Flow () , under Vapor-Liquid Equilibrium, is used to simulate evaporation and condensation to or from a vapor-liquid interface. It combines the functionality of the Single-Phase Flow Interface with functionality for mass transfer at vapor-liquid interfaces.

The Laminar Two-Phase Flow interface () , under Vapor-Liquid Equilibrium, is used to simulate evaporation and condensation to or from a vapor-liquid interface, and to track the position of the interface. It combines the functionality of the Single-Phase Flow Interface with functionality for mass transfer at vapor-liquid surfaces as well as functionality for tracking a moving vapor-liquid interface.

The Surface Reactions interface () models reactions involving surface adsorbed species and species in the bulk of a reacting surface. This interface is used on a model boundary, and is coupled to a mass transport interface active on a model domain. The interface can be used together with the Reacting Flow interfaces, and the Electrochemistry interfaces. The Electrochemistry interfaces require the addition of one of the Battery Design Module, the Corrosion Module, the Electrochemistry Module, the Electrodeposition Module, or the Fuel Cell & Electrolyzer Module. Predefined expressions for the growth velocity of the reacting surface makes it easy to set up models with moving boundaries.

The Transport of Diluted Species in Fractures interface () is used to model solute species transported along fracture surfaces where the thickness is very small compared to the other dimensions. Geometries like these are often hard to mesh. In this interface the fractures are defined by boundaries in the model geometry, circumventing the need for a mesh in the thin dimension. The interface allows you to define the average fracture thickness and also the porosity, for cases when the fracture is considered to be a porous structure. Different effective diffusivity models are available for such cases. The interface includes support for transport due to convection, diffusion, and dispersion, as well as chemical reactions.

SINGLE-PHASE FLOW

The Creeping Flow interface () is used to model flow at very low Reynolds numbers, in which case the inertial term in the Navier-Stokes equations can be neglected. Creeping flow, also referred to as Stokes flow, occurs in systems with high viscosity or small geometrical length scales, for example in microfluidics and MEMS devices.

The Laminar Flow interface () is used to model flow at low to intermediate Reynolds' numbers, and often in combination with mass transport and heat transfer. The interface solves the Navier–Stokes equations and assumes by default that a flow is incompressible. This simplifies the numerical scheme and provides fast and efficient flow simulations. You can also choose to model compressible flow in which case the density may depend on pressure, composition, and temperature. The interface supports compressible flow at speeds of less than Mach 0.3.

Another useful tool is the ability to describe other material properties such as density and viscosity by entering equations that describe these terms as a function of other parameters such as material concentration, pressure, or temperature. Many materials in the material libraries use temperature- and pressure-dependent property functions.

MULTIPHASE FLOW

The Mixture Model, Laminar Flow interface () models two-phase flow including a continuous liquid phase and a dispersed phase consisting of liquid droplets or solid particles. The interface allows for mass transfer between the two phases.

POROUS MEDIA AND SUBSURFACE FLOW

The Brinkman Equations interface () is used to model porous flow when the size of the interstices is larger; the Brinkman interface extends Darcy's law to describe the dissipation of the kinetic energy by viscous shear, similar to the Navier–Stokes equations. The interface includes the possibility to add a Forchheimer drag term, which simulates viscous drag in very open beds where turbulent drag becomes important. Forchheimer drag is sometimes called Ergun's equations. For very low speed flows or small geometrical length scales, you can also choose to neglect the inertial term (Stokes flow).

The Darcy's Law interface () is used to model fluid movement through interstices in a porous medium where a homogenization of the porous and fluid media into a single medium is done. Together with the continuity equation and equation of state for the pore fluid this interface can be used to model flows for which the pressure gradient is the major driving force. The penetration of reacting gases through a catalytic washcoat or membrane is a classic example for the use of Darcy's Law.

Darcy's law can be used in porous media where the fluid flow pattern is mostly influenced by the frictional resistance within the pores. Its use is within very slow flows, or media where the porosity is relatively small. Fluid penetration through

filters and packed beds are applications that are suitable to model with this interface.

The Free and Porous Media Flow, Brinkman interface () is useful for equipment that contain domains where free flow is connected to porous media, such as packed-bed reactors and catalytic converters. It should be noted that if the porous region is large in comparison to the free fluid region, and you are not primarily interested in results in the region of the interface, then you can always couple the Laminar Flow interface to the Darcy's Law interface, to make your overall model computationally cheaper.

The Free and Porous Media Flow, Darcy interface () provides such a coupling to model porous media flow connected to free flow domains. This multiphysics interface automatically couples the Laminar Flow interface with the Darcy's Law interface over their common boundary.

As always, the interface gives you direct access to defining, with either constants or expressions, the material properties that describe the porous media flow. This includes the density, dynamic viscosity, permeability, porosity, and matrix properties.

NONISOTHERMAL FLOW

The Nonisothermal Flow, Laminar Flow multiphysics interface () is primarily applied to model flow at low to intermediate Reynolds numbers in situations where the temperature and flow fields have to be coupled. A typical example is natural convection, where thermal buoyancy forces drive the flow.

The Brinkman Equations multiphysics interface () couples the Brinkman Equations interface to a Heat Transfer in Porous Media interface and automatically adds a Porous Material node under Materials in the model tree.

FLUID–STRUCTURE INTERACTION, FIXED GEOMETRY

The Fluid-Solid Interaction, Fixed Geometry () interface can be used to model phenomena where a fluid and a deformable solid structure affect each other. The interface models situations where the displacements of the solid are assumed to be small enough for the geometry of the fluid domain to be considered as fixed during the interaction.

HEAT TRANSFER

The various Heat Transfer interfaces include Heat Transfer in Fluids (), Heat Transfer in Solids (), Heat Transfer in Porous Media (), Heat Transfer in Packed Beds (), and account for conductive and convective heat transfer. These features interact seamlessly and can be used in combination in a single model.

The Physics Interface List by Space Dimension and Study Type

The table lists the physics interfaces available with this module in addition to those included with the COMSOL Multiphysics basic license.

PHYSICS INTERFACE	ICON	TAG	SPACE DIMENSION	AVAILABLE STUDY TYPE
 Chemical Species Transport				
Transport of Diluted Species ¹		tds	all dimensions	stationary; time dependent
Transport of Concentrated Species		tcs	all dimensions	stationary; time dependent
Chemistry		chem	all dimensions	stationary; time dependent
Reaction Engineering		re	0D	time dependent; stationary plug flow
Nernst–Planck Equations		npe	all dimensions	stationary; time dependent
Nernst–Planck–Poisson Equations		tds+es	all dimensions	stationary; time dependent; stationary source sweep; small-signal analysis, frequency domain
Electrophoretic Transport		el	all dimensions	stationary; stationary with initialization; time dependent; time dependent with initialization
Transport of Diluted Species in Porous Media		tds	all dimensions	stationary; time dependent
Transport of Concentrated Species in Porous Media		tcs	all dimensions	stationary; time dependent
Surface Reactions		sr	all dimensions	stationary (3D, 2D, and 2D axisymmetric models only); time dependent
Transport of Diluted Species in Fractures		dsf	3D, 2D, 2D axisymmetric	stationary; time dependent

PHYSICS INTERFACE	ICON	TAG	SPACE DIMENSION	AVAILABLE STUDY TYPE
 Reacting Flow				
Laminar Flow, Diluted Species ¹		—	3D, 2D, 2D axisymmetric	stationary; time dependent
Laminar Flow, Concentrated Species		—	3D, 2D, 2D axisymmetric	stationary; time dependent
 Reacting Flow in Porous Media				
Transport of Diluted Species		—	3D, 2D, 2D axisymmetric	stationary; time dependent
Transport of Concentrated Species		—	3D, 2D, 2D axisymmetric	stationary; time dependent
Transport of Diluted Species, Porous Catalyst		—	3D, 2D, 2D axisymmetric	stationary; time dependent
Transport of Concentrated Species, Porous Catalyst		—	3D, 2D, 2D axisymmetric	stationary; time dependent
Transport of Diluted Species, Packed Bed		—	3D, 2D, 2D axisymmetric	stationary; time dependent
Transport of Concentrated Species, Packed Bed		—	3D, 2D, 2D axisymmetric	stationary; time dependent
Transport of Diluted Species, Packed Bed, Shrinking Core Model		—	3D, 2D, 2D axisymmetric	stationary; time dependent
Transport of Diluted Species, Moving Bed		—	3D, 2D, 2D axisymmetric	stationary; time dependent
Transport of Concentrated Species, Moving Bed		—	3D, 2D, 2D axisymmetric	stationary; time dependent
Transport of Diluted Species, Moving Bed, Shrinking Core Model		—	3D, 2D, 2D axisymmetric	stationary; time dependent

PHYSICS INTERFACE	ICON	TAG	SPACE DIMENSION	AVAILABLE STUDY TYPE
 Nonisothermal Reacting Flow				
Brinkman Equations		—	3D, 2D, 2D axisymmetric	stationary; time dependent
Laminar Flow		—	3D, 2D, 2D axisymmetric	stationary; time dependent
 Dispersed Two-Phase Flow with Species Transport				
Laminar Flow		—	3D, 2D,	stationary; time dependent
 Vapor-Liquid Equilibrium				
Laminar Vapor Flow		—	3D, 2D, 2D axisymmetric	stationary; time dependent
Laminar Two-Phase Flow		—	3D, 2D, 2D axisymmetric	stationary; time dependent
 Precipitation and Crystallization				
Size-Based Population Balance		pbsb	all dimensions	stationary; time dependent
Precipitation in Fluid Flow		—	3D, 2D, 2D axisymmetric	stationary; time dependent
Precipitation		—	0D	stationary; time dependent
 Fluid Flow				
 Single-Phase Flow				
Creeping Flow		spf	3D, 2D, 2D axisymmetric	stationary; time dependent
Laminar Flow ¹		spf	3D, 2D, 2D axisymmetric	stationary; time dependent

PHYSICS INTERFACE	ICON	TAG	SPACE DIMENSION	AVAILABLE STUDY TYPE
 Porous Media and Subsurface Flow				
Brinkman Equations		br	3D, 2D, 2D axisymmetric	stationary; time dependent
Darcy's Law		dl	all dimensions	stationary; time dependent
Free and Porous Media Flow, Brinkman		fp	3D, 2D, 2D axisymmetric	stationary; time dependent
Free and Porous Media Flow, Darcy		—	3D, 2D, 2D axisymmetric	stationary; time dependent
 Nonisothermal Flow				
Brinkman Equations		—	3D, 2D, 2D axisymmetric	stationary; time dependent; stationary, one-way NITF; time dependent, one-way NITF
 Heat Transfer				
Heat Transfer in Fluids ¹		ht	all dimensions	stationary; time dependent
Heat Transfer in Solids and Fluids ¹		ht	all dimensions	stationary; time dependent
Heat Transfer in Porous Media		ht	all dimensions	stationary; time dependent
¹ This physics interface is included with the core COMSOL Multiphysics software but has added functionality for this module.				

Tutorial Model: NO_x and Ammonia Conversion in a Monolithic Reactor

Introduction

This tutorial model presents a detailed description of how to set up a model of a catalytic reactor for exhaust gas treatment. The example shows an application of the modeling strategy, described in the section [Chemical Reaction Engineering Simulations](#) and demonstrates through a series of simulations how an understanding of the catalytic reactor and its system can be improved. To do this, it uses a number of the interfaces and features found in the Chemical Reaction Engineering Module. Transport and thermodynamic properties are provided by the Thermodynamics feature under Global Definitions.

The system to be modeled is the selective reduction of harmful nitrogen oxides NO_x (NO and NO₂) into nitrogen (N₂) 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 (NH₃) to nitrogen.

In both of the beds there are unwanted side-reactions. In the first bed, NH₃ may react with oxygen instead of reducing NO_x. This means that the amount of injected ammonia must exceed the amount of NO_x, while not being so excessive as to release NH₃ to the atmosphere. In the second bed, ammonia should get oxidized into nitrogen, but may instead react to form NO_x. This is another reason to try and keep the injected amount of ammonia to a minimum.

The goals of the simulations are to find the optimal dosing of NH_3 , and to investigate the influence of engine load on the system. The engine load affects the gas temperature, amount of NO_x , and mass flow rate of the exhaust gas.



The exhaust aftertreatment system is contained in a box acting as a heat shield and protecting the catalysts and filters inside. The box is often installed next to the front wheel to be close to the engine. This position minimize the heat loss from the exhaust gases before they reach the catalysts, ensuring the highest conversion possible.

Tutorial Modeling Strategy

You may want to revisit the flowchart in [Figure 1](#) to follow the modeling strategy for this model as described next.

In short, two models, hereafter referred to as Single Channel Model, and Monolith Reactor Model, are set up.

The aim with the Single Channel model is to get an better understanding of the chemical kinetics in the system. To accomplish this, 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 the system for several different inlet temperatures, keeping the ammonia-to- NO_x 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- NO_x 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- NO_x is investigated. 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- NO_x ratio is kept constant, while the inlet conditions are varied between three engine load cases;

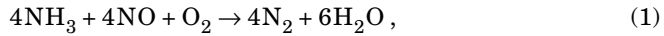
high load, intermediate load, and low load. This will reveal if the ammonia-to-NO_x ratio should be varied with engine load.

Having a better understanding of the reaction kinetics aids in the development of a more complex model. So, in the next step, the reaction kinetics implemented in the Single Channel Model are exported to the space-dependent Monolith Reactor Model. Here, the effect of temperature variations in the bed on the reaction rate and fluid flow can be investigated. This more advanced model reveals the necessary NH₃ dosing levels based on the working conditions of the catalytic reactor in the exhaust stream.

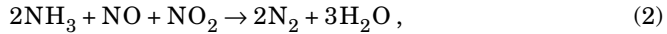
Chemistry

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

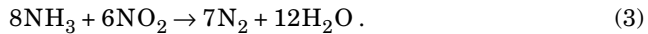
In the selective catalytic reduction bed, there are three desired SCR reactions that take place. These are the standard SCR reactions



the fast SCR reaction



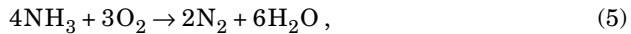
and the NO₂ SCR reaction



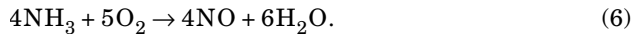
There is also the homogeneous oxidation of nitrogen monoxide into nitrogen dioxide



as well as two undesired reactions. These are 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](#):

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

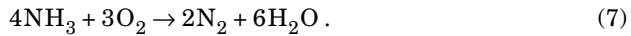
Here, G is a variable that accounts for the inhibition effects caused by adsorption of other species on the surface:

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

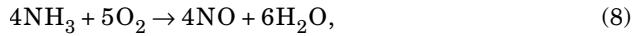
where K_i ($i=1-4$) follows an Arrhenius-type expression

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

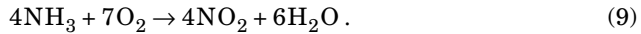
In the ammonia slip catalyst bed, there is one desired, two undesired reactions, and the homogeneous equilibrium reaction (4) that take place. The desired reaction is the oxidation of ammonia to form nitrogen:



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



and the oxidation of ammonia into nitrogen dioxide



Reaction 7 and 8 are the same chemical equations as Reaction 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:

$$r_9 = k_9 \frac{c_{\text{NH}_3} c_{\text{O}_2}}{G}. \quad (10)$$

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 minimal level of NH_3 required to reduce the NO_x present in the exhaust gas requires a reactor model accounting for changing reactant concentrations and system temperature.

From a mass transfer point of view, channels of the reactor monolith can be considered to be independent of each other. Therefore, it is reasonable to perform initial 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 given by:

$$\frac{dF_i}{dV} = R_i, \quad (11)$$

where F_i is the species molar flow rate (SI unit: mol/s), V represents the reactor volume (SI unit: m³), and R_i is the species net reaction rate (SI unit: mol/(m³·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):

$$F_i = v c_i, \quad (12)$$

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):

$$v = uA. \quad (13)$$

The energy balance for the ideal reacting gas is:

$$\sum_i F_i C_{p,i} \frac{dT}{dV} = Q_{\text{ext}} + Q, \quad (14)$$

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 the heat of reaction (SI unit: J/mol), 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 11–Equation 14 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.

Results for the Single Channel Model

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 3.

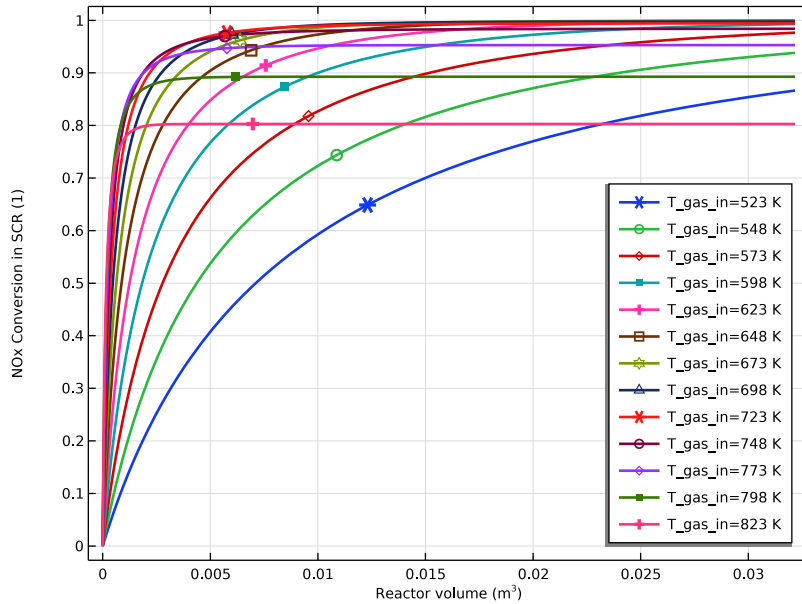


Figure 3: NO_x conversion along the reactor axis as a function of inlet temperature, for an $\text{NH}_3:\text{NO}_x$ ratio equal to 1.3, in the selective catalytic reduction bed.

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 4 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,

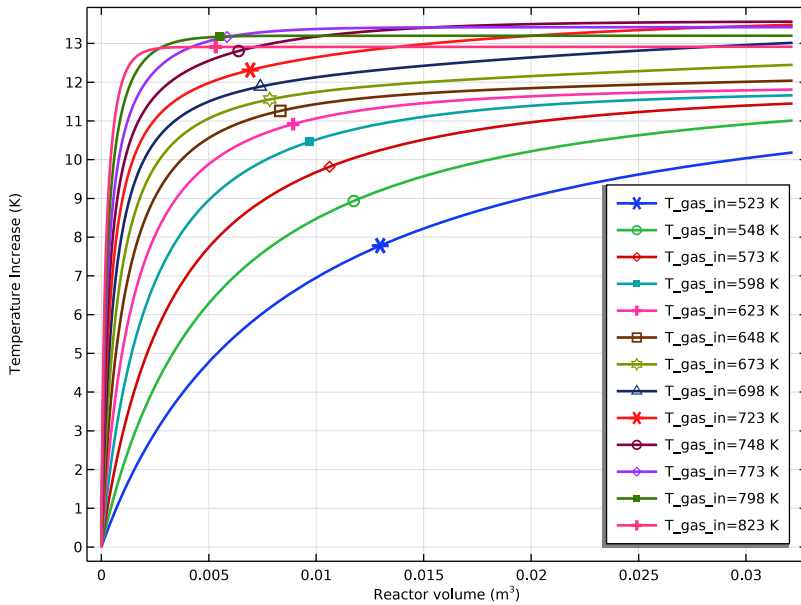


Figure 4: Temperature along the reactor axis as a function of inlet temperature in the selective catalytic reduction bed. $\text{NH}_3:\text{NO}_x$ ratio equal to 1.3

The optimal temperature operating window, defined as the temperatures giving maximum conversion of NO_x , is 620–720K for the SCR bed at an $\text{NH}_3:\text{NO}_x$

ratio equal to 1.3. The conversion of NO_x is close to complete at this temperature. This is seen in [Figure 5](#).

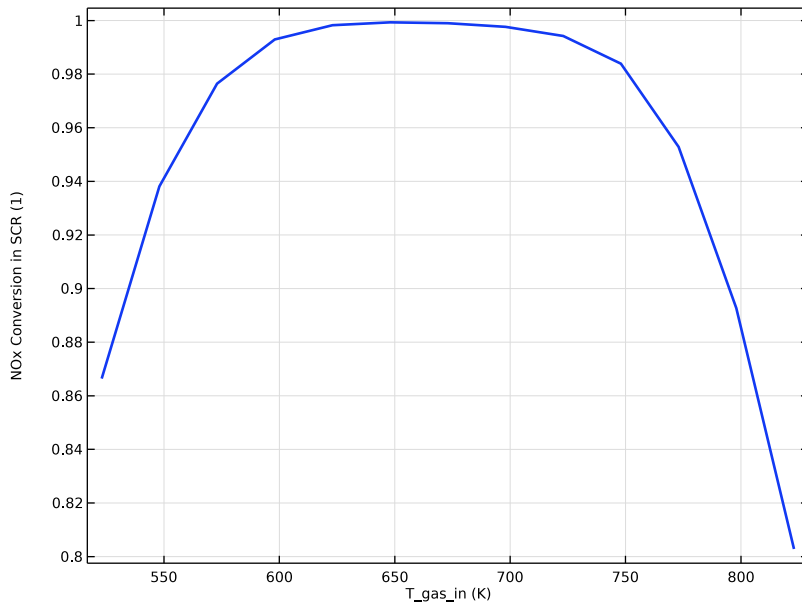


Figure 5: Final conversion of NO_x in the selective catalytic reduction (SCR) bed as a function of inlet gas temperature. The NH₃:NO_x ratio is equal to 1.3.

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 6](#) 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.

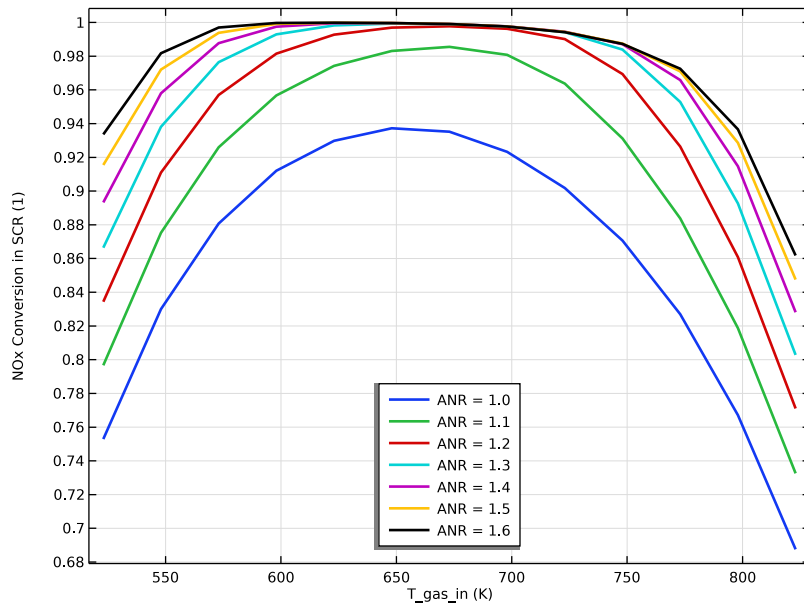


Figure 6: Final conversion of NO_x in the selective catalytic reduction (SCR) bed as a function of inlet gas temperature and NH₃:NO_x ratio.

The conversion of ammonia as a function of ANR and inlet gas temperature is seen in Figure 7. Complete conversion of ammonia is reached for all ANR at inlet gas temperatures above 750 K.

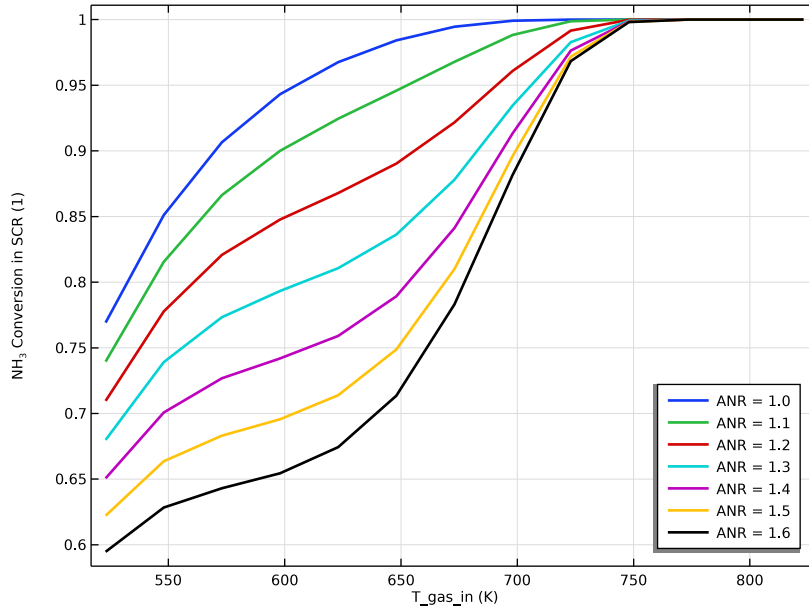


Figure 7: Final conversion of ammonia in the selective catalytic reduction (SCR) bed as a function of inlet gas temperature and $\text{NH}_3\text{:NO}_x$ ratio.

SINGLE CHANNEL MODEL

The results from the SCR-bed model revealed that the optimal conversion window for NO_x is at a lower temperature than that of ammonia. We also saw that the ammonia-to- NO_x ratio needs to be kept above 1.2 to reach complete conversion of NO_x . 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,

single channel model is therefor investigated. Figure 8 shows the molar fraction of ammonia and NOx along a single monolith channel in each bed.

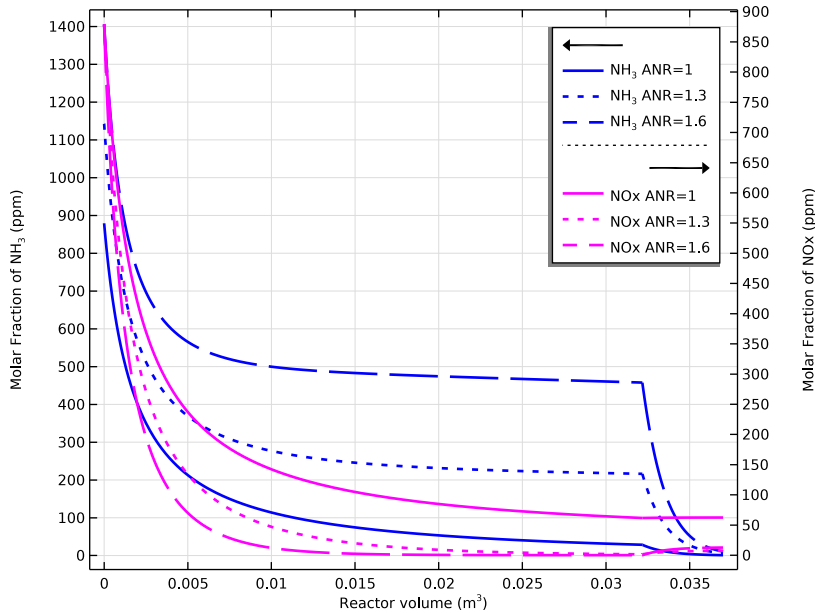


Figure 8: Molar fraction of ammonia and NOx in the dual bed, single channel system along the reactor axis. The $\text{NH}_3\text{:NOx}$ ratio varies from 1 to 1.6.

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, single channel system is seen in Figure 9.

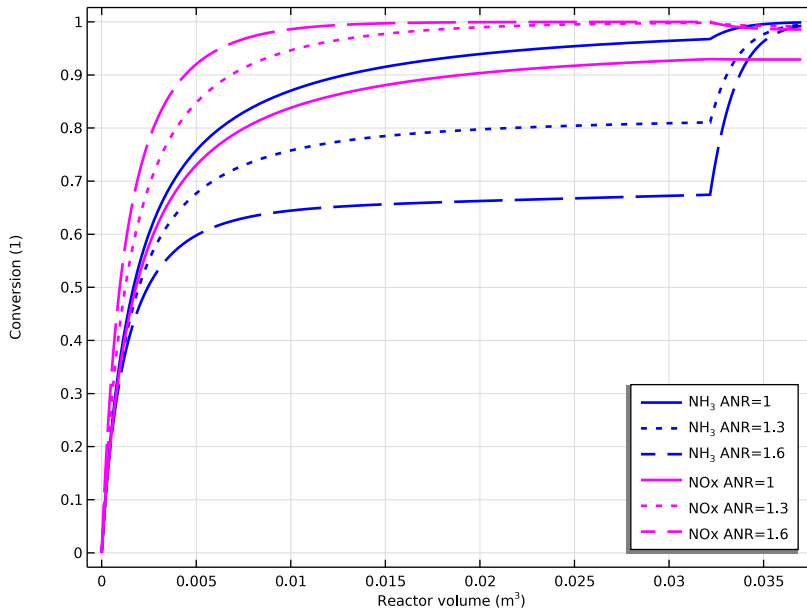


Figure 9: Conversion of ammonia and NOx in the dual bed system along the reactor axis. The $\text{NH}_3\text{:NO}_x$ ratio varies from 1 to 1.6.

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:

INLET GAS CONDITIONS FOR EACH ENGINE LOAD CASE

	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 NOx, 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, and low NOx from

the engine. Figure 10 shows the molar fraction for these three load cases, and an ANR of 1.3.

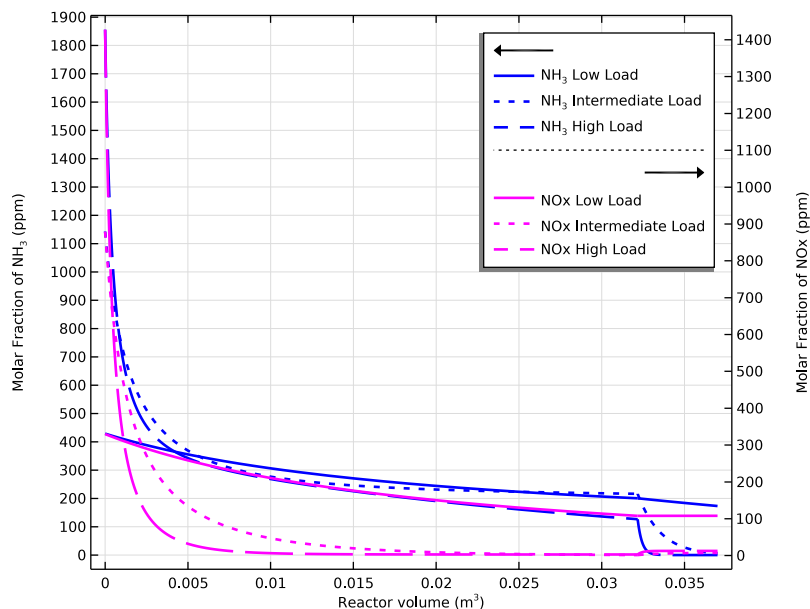


Figure 10: Molar fraction of NOx and ammonia as a function of axis position in the reactor. ANR equals 1.3, and the results from the three engine load cases are shown.

This figure reveals that the highest emissions of both NOx 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 NOx 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 NOx emission is achieved for the intermediate load. The high load would give lower NOx emissions if the ANR is decreased, as some of the NOx 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 single channel system for each of the three engine load cases.

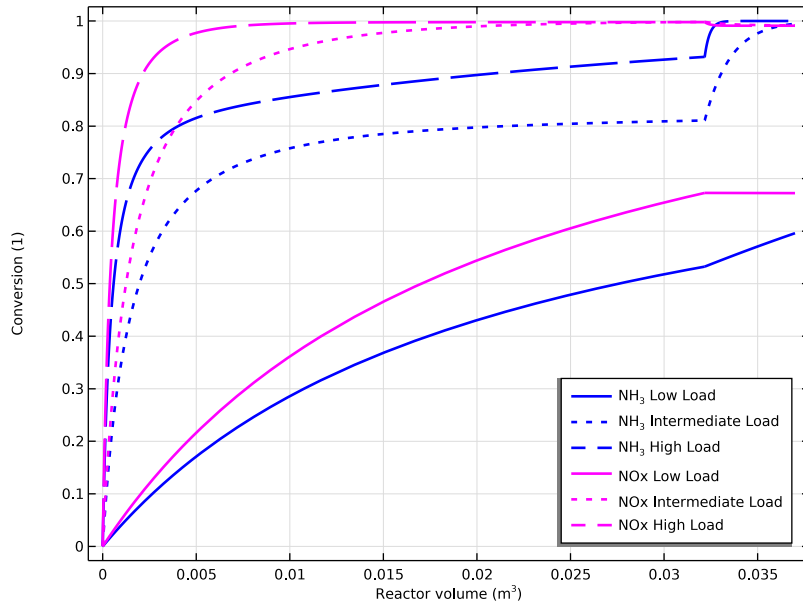


Figure 11: Conversion of ammonia and NOx for the three engine load cases and an ANR equal to 1.3.

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.

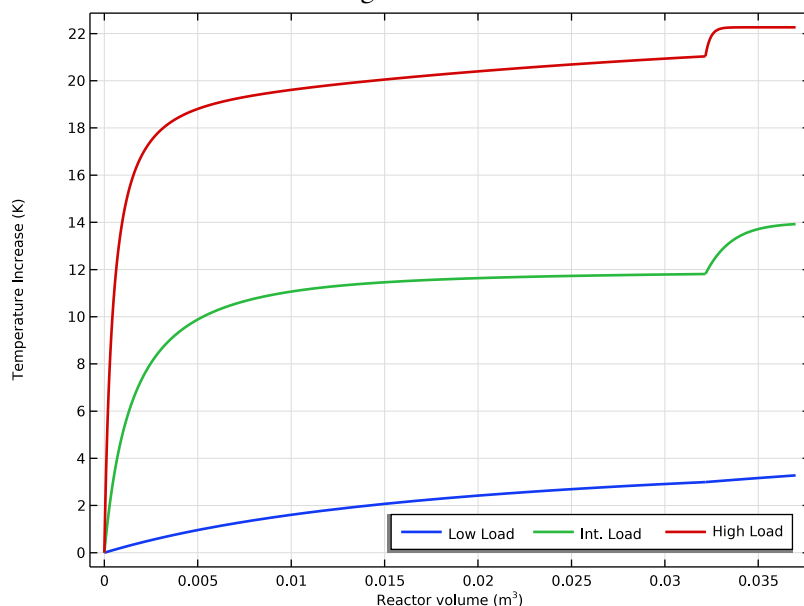


Figure 12: Temperature increase in the reactor for the three engine load cases and an ANR equal to 1.3.

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 $\text{NH}_3\text{:NOx}$ ratio of 1.3 appears appropriate for the extended model.

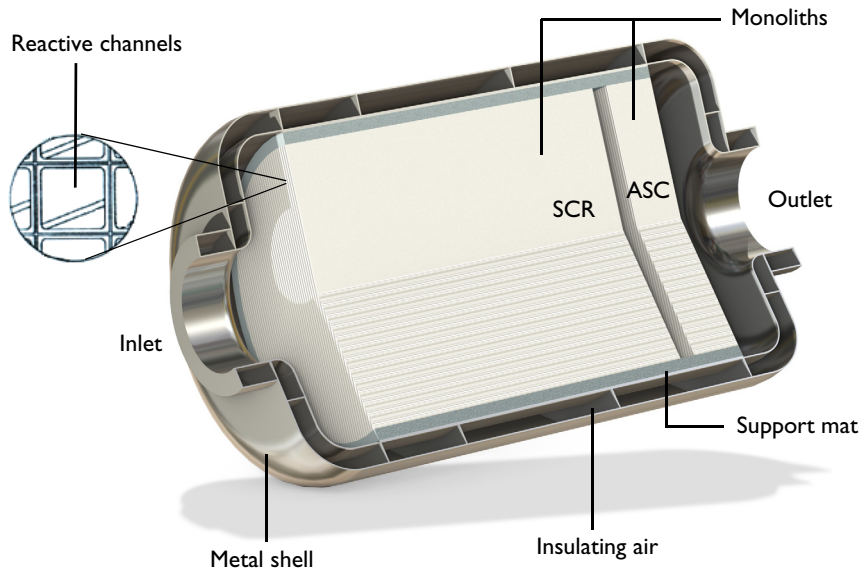
Monolith Reactor Model

It is clear from the Single Channel Model that temperature plays a central role in affecting the optimal dosing of NH_3 . As the temperature distribution is likely to vary from channel to channel in a catalytic converter, a full monolithic reactor model is required.

MODEL GEOMETRY

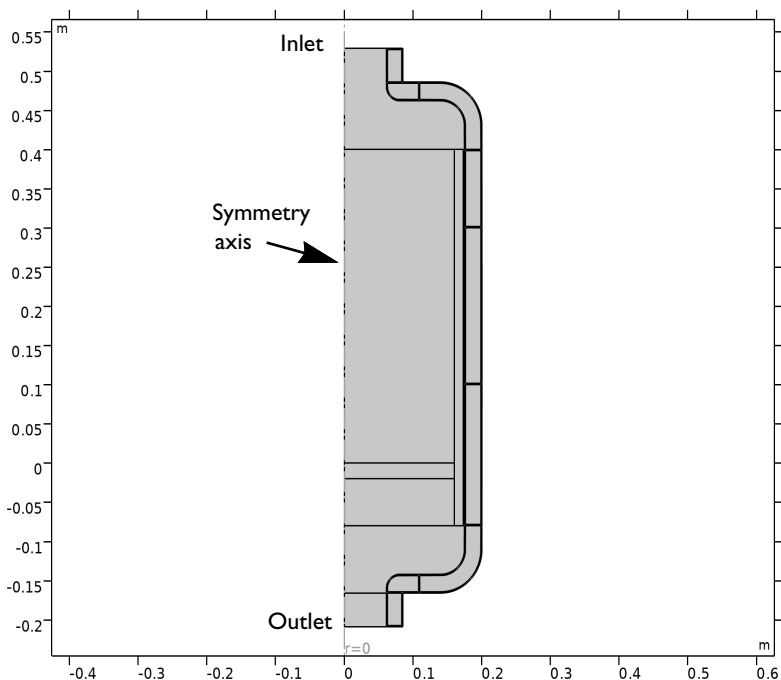
The modeled reactor consists of a metal shell that protects and insulates the two catalysts placed inside. Each catalytic bed consists of a monolithic support that is loaded with active catalytic material. These two porous domains are modeled as one material in this model. The catalysts are placed in series, wrapped in a porous supportive mat, and contained in a metal can. The supportive mat protects the

catalysts from vibrations and holds them in place. Each monolith consists of reactive channels separated by impermeable walls. The first bed in the reactor is 0.4 m long, and the second bed is 0.06 m long. They are placed with a small gap between. Both beds have a diameter of 0.32 m. The void fraction of the catalyst beds are 0.75. A seal is placed at the inlet of the support mat to prevent erosion of the mat, as well as bypassing of reactive gas through the mat. This seal is included as a boundary condition during simulation, and not a detail in the geometry. An illustration of the modeled system is found below.



The exhaust gas passes through the channels in the monolithic beds in the reactor.

The reactor is symmetric in its design which gives the geometry seen here.



Symmetry reduces the modeling domain.

MODEL EQUATIONS AND ASSUMPTIONS

In this example a pseudo homogeneous approach is used to model the hundreds of channels present in the monolith reactor. As no mass is exchanged between channels, each channel is described by 1D mass transport equations. Furthermore, fully developed laminar flow in the channels is assumed, such that the average flow field is proportional to the pressure difference across the reactor. The fluid flow transports mass and energy only in the channel direction. The energy equation describes the temperature of the reacting gas in the channels, as well as the conductive heat transfer in the solid parts of the monolith structure. As the temperature affects not only the reaction kinetics but also the density and viscosity of the reacting gas, the energy equation is what really connects the channels in the reactor structure turning this into a space-dependent model.

Reaction Kinetics

The chemical equations and rate expressions are the same as those in the [Chemistry](#) section for the Single Channel Model.

Mass Transport

The mass balances describing transport and reaction in the reacting channels are given by diffusion-convection equations at steady state:

$$\nabla \cdot (-D_i \nabla c_i) + \mathbf{u} \cdot \nabla c_i = R_i \quad (15)$$

In Equation 15, D_i denotes the diffusion coefficient (SI unit: m^2/s), c_i is the species concentration (SI unit: mol/m^3), and $\mathbf{u}$ equals the velocity vector (SI unit: m/s). The term R_i (SI unit: $\text{mol}/(\text{m}^3 \cdot \text{s})$) corresponds to the species' rate expression.

Mass transport is only allowed in the direction of the channels, corresponding to direction of the z -axis in the 2D-axisymmetric geometry used in this example. For the diffusive transport, this is accomplished by setting the x and y -components of the diffusivity matrix to zero. The pressure-driven flow in the monolith is also defined in the direction of the z -axis, hereby restricting the convective mass transport to the channel direction as well. Each monolith channel thus behaves as a 1D plug flow model with included diffusion. These separate channel models are connected through the heat transfer equations for the reactor monolith.

Species concentrations are defined at the reactor inlet boundaries:

$$c = c_{\text{in}}.$$

At the outlet, use the Outflow condition:

$$\mathbf{n} \cdot (-D \nabla c) = 0.$$

Fluid Flow

Assuming there is fully developed laminar flow in the channels, the average flow field is proportional to the pressure difference across the reactor. The flow of reacting gas through the monolith can then be modeled using Darcy's Law with the following governing equations:

$$\nabla \cdot (\rho \mathbf{u}) = 0 \quad (16)$$

$$\mathbf{u} = -\frac{\kappa}{\mu} \nabla p \quad (17)$$

The monolith is treated as a porous matrix with the effective permeability κ (SI unit: m^2). Similarly to the diffusivity, the x - and y -components of the permeability matrix are set to zero. The density, ρ (SI unit: kg/m^3), and viscosity, μ (SI unit: $\text{Pa} \cdot \text{s}$), of the gas are assumed to be well represented by the temperature-dependent properties of nitrogen, as only relatively small concentrations of other gases are present.

Pressure conditions are set at the reactor inlet and outlet boundaries.

Heat Transfer

A single temperature equation describing the heat transfer in the porous monolith reactor can be written as:

$$(\rho C_p)_{\text{eff}} \frac{\partial T}{\partial t} + \rho_f C_{pf} \mathbf{u} \cdot \nabla T = \nabla \cdot (k_{\text{eff}} \nabla T) + Q \quad (18)$$

For the stationary case this reduces to:

$$\rho_f C_{pf} \mathbf{u} \cdot \nabla T = \nabla \cdot (k_{\text{eff}} \nabla T) + Q \quad (19)$$

where ρ_f (SI unit: kg/m^3) is the fluid density, C_{pf} (SI unit: $\text{J}/(\text{kg}\cdot\text{K})$) is the fluid heat capacity, and k_{eff} (SI unit: $\text{W}/(\text{m}\cdot\text{K})$) is the equivalent thermal conductivity. Furthermore, $\mathbf{u}$ (SI unit: m/s) is the fluid velocity field derived by the fluid flow interface. Q (SI unit: W/m^3) is the heat source due to exothermic chemical reactions:

$$Q = -\sum_j H_j r_j. \quad (20)$$

Above, H_j (SI unit: $\text{J}/(\text{mol}\cdot\text{K})$) is the heat of reaction for reaction j , and r_j is the reaction rate for said reaction.

The effective conductivity of the solid-fluid system, k_{eff} , is related to the conductivity of the solid, k_s , and to the conductivity of the fluid, k_f , by:

$$k_{\text{eff}} = \Theta_s k_s + \Theta_f k_f. \quad (21)$$

In [Equation 21](#), Θ_s denotes the solid material's volume fraction, which is related to the volume fraction of the fluid Θ_f by:

$$\Theta_f + \Theta_s = 1. \quad (22)$$

[Equation 19](#) is the equation set up by the Heat Transfer interface for a fluid domain. For the solid monolith, only heat transfer by conduction applies:

$$-\nabla \cdot (k_s \nabla T) = 0, \quad (23)$$

where k_s (SI unit: $\text{W}/(\text{m}\cdot\text{K})$) is the thermal conductivity for the solid walls. For the extruded monolith material, the thermal conductivity is anisotropic.

The heat transfer in the porous support mat is also described by [Equation 19](#) and [23](#). Contrary to the monoliths, the support mat has isotropic thermal conductivity. The same is true for the solid metal walls in the reactor.

The temperature is specified at the reactor inlet walls:

$$T = T_0,$$

and the Inflow condition; that is,

$$-\mathbf{n} \cdot \mathbf{q} = \rho \Delta H \mathbf{u} \cdot \mathbf{n}$$

is used at the inlet of the first bed. ΔH (SI unit: J/(kg)) is the sensible enthalpy. At the outlet of the second bed, use the Outflow condition:

$$\mathbf{n} \cdot (k \nabla T) = 0.$$

For the external reactor walls, the heat flux through the boundaries is given by

$$\mathbf{q}_m \cdot \mathbf{n} = h(T - T_{\text{amb}}),$$

where h (SI unit: W/(m²·K)) denotes the heat transfer coefficient, and T_{amb} (K) equals the ambient temperature.

As mentioned, the temperature affects not only reaction kinetics but also the density and viscosity of the reacting gas. In this way the heat transfer equation connects the channels in the reactor structure.

Thermodynamic and Transport Properties

Accurate thermodynamic data is required as input to energy balance equations, both in the Single Channel Model (plug flow model, (Equation 14)) and the Monolith Reactor Model (Equation 19). In addition to thermodynamic properties, the model equations also require transport properties to describe the space-dependent reactor model.

The Thermodynamics feature provides all necessary properties for the simulation. Different models are available for thermal and transport property calculations (see [Thermodynamic Models and Theory](#)). In this system, thermodynamic properties are calculated based on the ideal gas law while transport properties such as diffusivity, viscosity, and thermal conductivity are calculated from [Fuller–Schettler–Giddings](#), [Brokaw](#), and [Kinetic Theory](#), respectively.

Results for the Monolith Reactor Model

The system conditions used in this monolith reactor model is the same as those used for the single channel model. Three [Solid](#) are investigated, with a fixed ammonia-to-NO_x ratio of 1.3.

[Figure 13](#) shows the molar fraction of NH₃, NO, and NO₂ in the two catalyst beds for the low engine load case. The effect of the radial temperature gradient is clearly visible as the conversion decreases close to the edge. The temperature for the low engine load case is below the optimal temperature for the SCR reactor, see

Figure 5. The low temperature results in low conversion of both NO_x and ammonia.

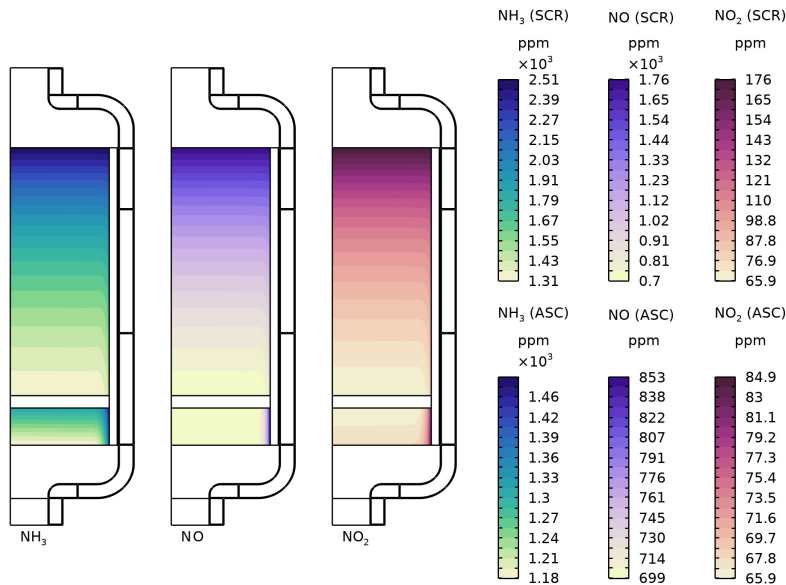


Figure 13: Molar fraction of ammonia, nitrogen monoxide, and nitrogen dioxide in the reactor. Low engine load, and NH₃:NO_x equal to 1.3. Fluid flow from top to bottom.

Figure 14 illustrates the result for the intermediate engine load case. At this increased temperature, the conversion increases in the reactor. Higher mass flow

rate and higher heat source due to increased conversion, gives smaller radial temperature gradient.

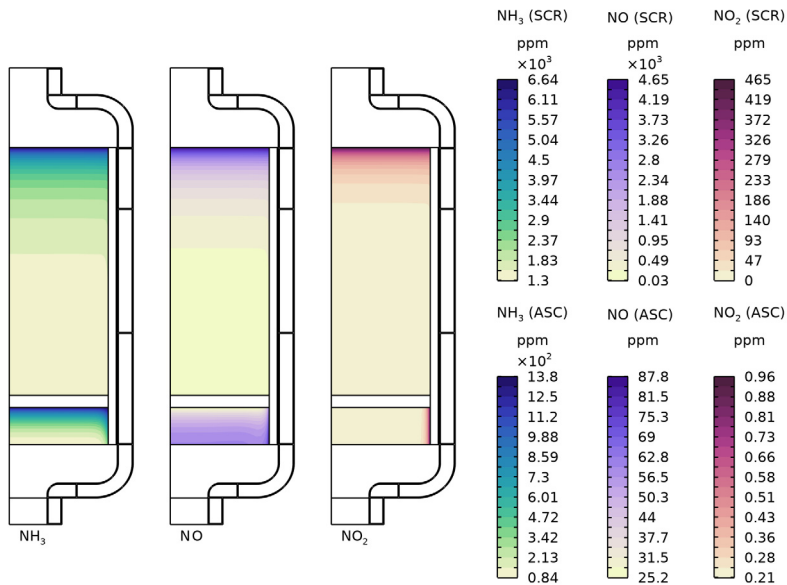


Figure 14: Molar fraction of ammonia, nitrogen monoxide, and nitrogen dioxide in the reactor. Intermediate engine load, and $\text{NH}_3:\text{NO}_x$ equal to 1.3. Fluid flow from top to bottom.

Figure 15 shows the results for the high engine load case..

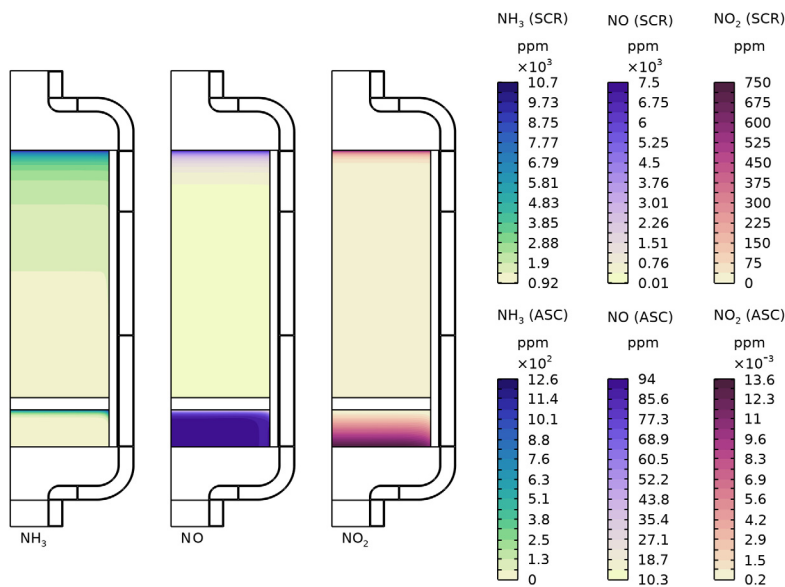


Figure 15: Molar fraction of ammonia, nitrogen monoxide, and nitrogen dioxide in the reactor. High engine load, and NH₃:NO_x equal to 1.3. Fluid flow from top to bottom.

The radial temperature gradient has less influence at increased space velocities. For the highest load case, the radial concentration difference is thus lower. Due to the high temperature, the activity of both beds are high. This results in the lowest ammonia emission among the three cases. During oxidation of ammonia in the ASC, the side reactions produce NO_x, resulting in a lower NO_x conversion than for the intermediate load case. At high engine loads, the ammonia-to-NO_x ratio should probably be lower than for the intermediate load.

Figure 16 illustrates the gas velocity, pressure, and temperature in the beds for the highest engine load.

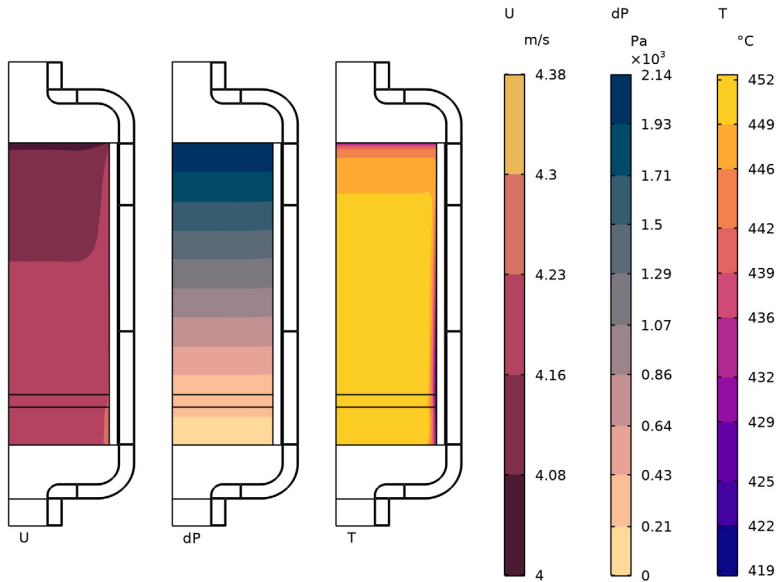


Figure 16: Gas velocity, pressure drop, and temperature in the reactor for the high engine load case. NH_3/NO_x equal to 1.3. Fluid flow from top to bottom.

The effect of temperature on conversion is seen in Figure 17. In this figure, the conversion is plotted both along the central symmetry axis, and along the edge of the monoliths. For a high engine load, the conversion does not vary significantly

with the position in the reactor, but for lower engine loads, the conversion differs significantly.

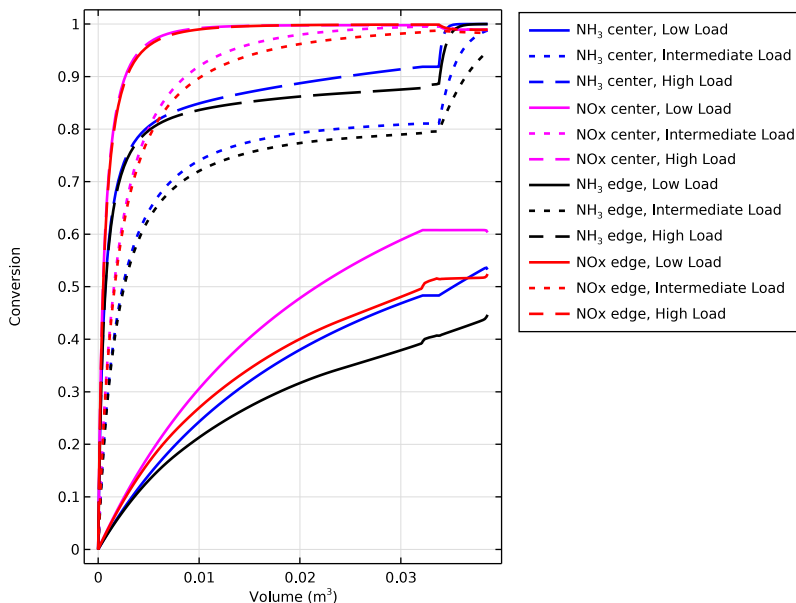


Figure 17: Conversion of ammonia and NOx along the center line, as well as along the monolith edge. All three engine load cases. $\text{NH}_3:\text{NOx}$ equal to 1.3.

The temperature differences along the reactor axis, at the center of the reactor, and at the edge of the beds, are seen in Figure 18. Close to the inlet of the first bed, the temperature increases both at the center and along the SCR edge. This is due to the exothermic reactions. After the first rapid temperature increase, the increase in temperature is slower, and at the edge of the first bed, the temperature instead decreases due to heat flux to the surroundings. For the high and intermediate engine load cases, the slip of ammonia from the first bed creates a significant temperature increase when this ammonia is oxidized in the second bed. For the low engine case, the activity is too low to create a temperature increase. At the bed edge, the heat flux to the surrounding decreases the temperature in the first bed,

decreasing the ammonia conversion rate, which creates an even larger temperature increased during ammonia oxidation in the second bed.

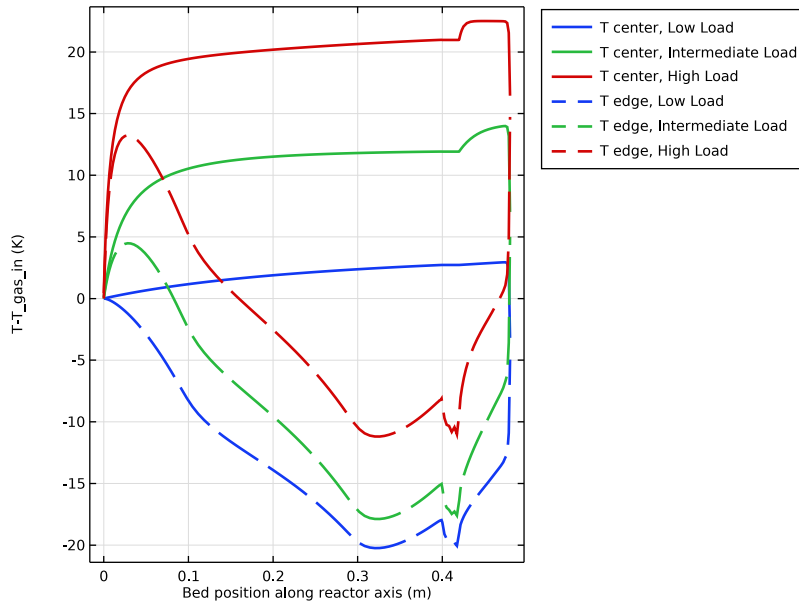


Figure 18: Temperature difference along the reactor axis, both at the center of the reactor, and at the edge of the monoliths. All three engine load cases. $\text{NH}_3:\text{NO}_x$ equal to 1.3.

Finally, the average values of ammonia and NO_x molar fractions were derived both along the outlet of the first bed, as well as along the outlet of the second bed. The values are found in Table 1.

TABLE 1: MOLAR FRACTIONS FOR AMMONIA AND NO_x OUT FROM EACH BED, FOR EACH ENGINE LOAD CASE

	Low load	Intermediate load	High load
y_{NH_3} out from first bed	1320 ppm	1299 ppm	932 ppm
y_{NH_3} out from second bed	1190 ppm	99.01 ppm	0 ppm
y_{NO_x} out from first bed	774 ppm	24 ppm	15 ppm
y_{NO_x} out from second bed	775.0 ppm	54 ppm	78 ppm

From the results in Table 1 it is clear that for an ammonia-to- NO_x ratio of 1.3, the exhaust gases from the truck will contain the least ammonia at high load, and the least NO_x at intermediate load.

With this model we have shown that in order to get low exhaust levels for both ammonia and NO_x, the injected amount of ammonia needs to be adjusted as a function of engine load.

The information from this monolith reactor model can also be used to investigate other aspects of the reacting system. For example, the results can be compared to other results from prototypes or even real monolith reactors, and material properties, such as the permeability constant, can be fine-tuned. Different operating conditions, such as when the automobile accelerates and decelerates, can be simulated. Alternative catalysts and designs can also be investigated.

Summary

The Chemical Reaction Engineering Module is used to perform two different levels of analysis concerning the reduction of NO_x in a monolithic reactor:

- **Single Channel Model** — With a simple plug flow reactor model explore the reaction kinetics and narrow down the conditions that promote selectivity toward NO_x reduction. The tuning of the dosage is improved by performing the modeling in several steps; that is, by first isolating the impact of temperature and then adding the impact of ammonia.
- **Monolith Reactor Model** — testing the reactor operating conditions in a full reactor representation, noting the space-dependent effect due to coupling between monolith channels.

This study revealed that the ammonia-to-NO_x ratio should be varied with engine load. A reactant ratio NH₃:NO of approximately 1.3 is found to be close to optimal for an intermediate engine load, but at higher loads this ratio could be decreased. At low engine load, the temperature is too low to give acceptable NO_x reduction.

The modeling strategy used in this example has several advantages. Starting with fast simulations using easy to set up models makes it easier to identify and narrow down the process condition envelope before moving to more advanced and computationally demanding models. The sequential modeling approach also helps to identify when and how effects such as temperature dependency and space dependency come into play. This deepened system understanding leads to efficient model setup and solution strategies. Going from perfectly mixed conditions to full space dependency also puts you in the position to decide on what level of detail that is needed for the particular system.

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 and 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.

Note on the Models

The following step-by-step instructions guide you through the process to set up and solve the two models that simulate the catalytic reduction of NO_x and ammonia in a monolith reactor. The first model, Single Channel Model, makes use of a simple plug flow reactor model. The second model, Monolith Reactor Model, accounts for the monolithic reactor, coupling mass transport to heat transfer and fluid flow.

As an option to first build the Single Channel Model, you can open the completed model file for the Single Channel Model and proceed directly with the setup of the Monolith Reactor Model. See [Modeling Instructions: Monolith Reactor Model](#) for further details.

Both the Single Channel Model and the Monolith Reactor Model are available in the Application Libraries, see `monolith_kinetics.mph` and `monolith_reactor.mph`, respectively.

Here follows the step-by-step instructions guide to how to build the Single Channel Model and the Monolith Reactor Model.

Modeling Instructions: Single Channel Model

By following these steps you will be able to set up the Single Channel Model.

Model Wizard

Note: These instructions are for the user interface on Windows but apply, with minor differences, also to Linux and macOS.

- 1 To start the software, double-click the COMSOL icon on the desktop. When the software opens, choose to use the Model Wizard to create a new COMSOL Multiphysics model, or choose Blank Model to create one manually. For this tutorial, click the Model Wizard button.

If COMSOL Multiphysics is already open, start the Model Wizard by choosing New  from the File menu and then click Model Wizard .

The Model Wizard guides you through the first steps of setting up a model. The next window lets you choose the dimension of the modeling space.

- 2 In the Select Space Dimension window click the 0D  button.
- 3 In the Select Physics tree, expand the Chemical Species Transport node. Then double-click Reaction Engineering  to add it to the Added physics interfaces list. Alternatively, right-click Reaction Engineering  and choose Add Physics .
- 4 Click Study . In the Select Study tree, under Preset Studies for Selected Physics Interfaces, select Stationary Plug Flow .
- 5 Click Done .

Parameters

Start by importing 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.

Note: The location of a file is based on the installation. For example, if the installation is on your hard drive, the file path might be similar to
C:\Program Files\COMSOL\COMSOL64\Multiphysics\applications\.

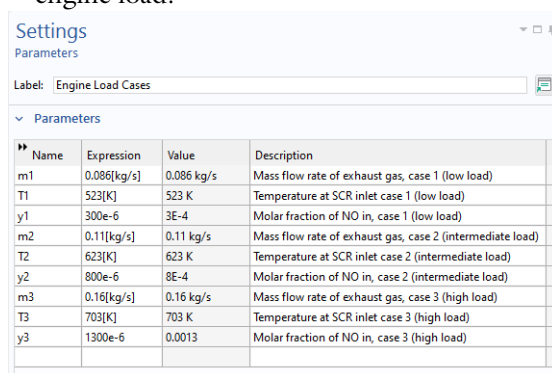
PARAMETERS: ENGINE LOAD CASES

1 In the Home toolbar, click Parameters  and choose Parameter 1 .

Note: On Linux and macOS, the Home toolbar refers to the specific set of controls near the top of the Desktop.

2 In the Settings window under Parameters, click the Load from File button .

3 Browse to the file `monolith_kinetics_engine_load_cases_parameters.txt` in the application library folder on your computer, `Chemical_Reaction_Engineering_Module\Tutorials`. Double-click to add or click Open. The parameters from the txt-file are added to the table. The loaded file contains mass flow rates, nitrogen monoxide concentration, 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.



The screenshot shows the 'Settings' window with the 'Parameters' tab selected. A text field labeled 'Label' contains 'Engine Load Cases'. Below it, a table lists parameters for three engine load cases: low, intermediate, and high. The table has four columns: Name, Expression, Value, and Description.

Name	Expression	Value	Description
m1	0.086[kg/s]	0.086 kg/s	Mass flow rate of exhaust gas, case 1 (low load)
T1	523[K]	523 K	Temperature at SCR inlet case 1 (low load)
y1	300e-6	3E-4	Molar fraction of NO in, case 1 (low load)
m2	0.11[kg/s]	0.11 kg/s	Mass flow rate of exhaust gas, case 2 (intermediate load)
T2	623[K]	623 K	Temperature at SCR inlet case 2 (intermediate load)
y2	800e-6	8E-4	Molar fraction of NO in, case 2 (intermediate load)
m3	0.16[kg/s]	0.16 kg/s	Mass flow rate of exhaust gas, case 3 (high load)
T3	703[K]	703 K	Temperature at SCR inlet case 3 (high load)
y3	1300e-6	0.0013	Molar fraction of NO in, case 3 (high load)

4 Rename the parameter node by editing the label text field. Rename it to Parameters: Engine Load Cases.

Use the global feature Parameter Case to specify the load cases. By using this feature, it is even easier to set up a Parametric Sweep later. A Parametric Sweep feature is used when solving the same system with different parameter values.

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 file, but you can also type them in directly in the table.

Variables

VARIABLES: REACTION KINETICS SCR

- 1 In the Model Builder window, under Component 1 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. One way to find the generated variable names is shown in [Equation View](#) below.

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`.

Thermodynamics

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, NO_2 , 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.

GAS SYSTEM

- 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_2H_4 since it is not needed, then add the rest of the species for this model.

SPECIES 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.

In the Reaction Engineering toolbar, click  Thermodynamics and choose Thermodynamic System. This opens the Thermodynamic System Wizard which is used to define a system, including phase and species, and to set up thermodynamics and transport properties models.

SELECT SYSTEM

- 1 In the first step in the wizard, keep Gas as the Selected system. Click Next  in the window toolbar.

SELECT SPECIES

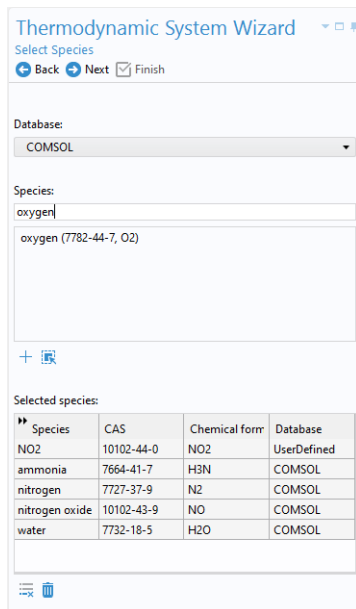
- 1 In the Select Species window, choose User defined from the Database list.
- 2 In the Species list, select NO2 (10102-44-0, NO2).
- 3 Click  Add Selected.
- 4 From the Database list, choose COMSOL.
- 5 In Select Species window, type the name of the remaining gas species that are present in the reactor system and Add  them to the Selected species table. Alternatively, it is also possible to double-click or press Enter to add species. Add ammonia, nitrogen, nitrogen oxide, oxygen, and water. Click Next .

SELECT THERMODYNAMIC MODEL

- 1 In the Select Thermodynamic Model, keep Ideal gas as Gas phase model.

As an option, check the Advanced options checkbox to select transport properties for later use in the space-dependent model. For now, keep the default selection by leaving the box cleared.

- 2 Click Finish .



Thermodynamic System Wizard

Select Species

Back Next Finish

Database:
COMSOL

Species:
oxygen

oxygen (7782-44-7, O2)

+ 

Selected species:

Species	CAS	Chemical form	Database
NO2	10102-44-0	NO2	UserDefined
ammonia	7664-41-7	H3N	COMSOL
nitrogen	7727-37-9	N2	COMSOL
nitrogen oxide	10102-43-9	NO	COMSOL
water	7732-18-5	H2O	COMSOL

In the Settings window it is possible to review all the properties of the created Gas System .

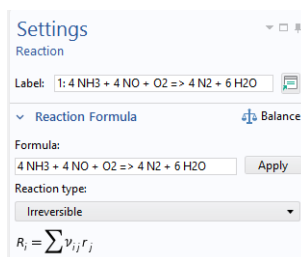
Reaction Kinetics for the Selective Catalytic Reduction (SCR) Catalyst

Now define the chemical reactions. First, type in the global reaction formula for the standard SCR reaction. The Reaction feature will automatically interpret the chemical equation and suggest reaction rates based on the mass action law (stoichiometry).

(1) STANDARD SCR: $4 \text{ NH}_3 + 4 \text{ NO} + \text{O}_2 \Rightarrow 4 \text{ N}_2 + 6 \text{ H}_2\text{O}$

- 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 $4\text{NH}_3+4\text{NO}+\text{O}_2\Rightarrow 4\text{N}_2+6\text{H}_2\text{O}$.
- 4 Click Apply to generate the Reaction node as well as one Species node for each of the species in the Reaction Formula.

 (1) Standard SCR: $4 \text{ NH}_3 + 4 \text{ NO} + \text{O}_2 \Rightarrow 4 \text{ N}_2 + 6 \text{ H}_2\text{O}$
 Species: NH_3
 Species: NO
 Species: O_2
 Species: N_2
 Species: H_2O



Settings
Reaction

Label: 1: 4 NH3 + 4 NO + O2 => 4 N2 + 6 H2O

Reaction Formula  Balance

Formula:
4 NH3 + 4 NO + O2 => 4 N2 + 6 H2O 

Reaction type:
Irreversible

$R_i = \sum_j \nu_{ij} r_j$

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_{NH_3} is defined in a Variables feature.

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

- 6 In the r_j text field, type $\text{re.kf_1*re.c_N0*re.c_O2*re.c_NH3}/(1+\text{K_NH3*re.c_NH3})$.

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

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

- 8 Locate the Rate Constants section. Select the Use Arrhenius expressions checkbox.

- 9 In the A^f text field, type $A1_SCR$.

- 10 In the E^f text field, type $E1_SCR$.

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

- 11 In the Label text field, type (1) Standard SCR: $4 \text{ NH}_3 + 4 \text{ NO} + \text{O}_2 \Rightarrow 4 \text{ N}_2 + 6 \text{ H}_2\text{O}$.

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: $2 \text{ NH}_3 + \text{NO} + \text{NO}_2 \Rightarrow 2 \text{ N}_2 + 3 \text{ H}_2\text{O}$

- 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 $2 \text{ NH}_3 + \text{NO} + \text{NO}_2 \Rightarrow 2 \text{ N}_2 + 3 \text{ H}_2\text{O}$.
- 4 In the Label text field, type (2) Fast SCR: $2 \text{ NH}_3 + \text{NO} + \text{NO}_2 \Rightarrow 2 \text{ N}_2 + 3 \text{ H}_2\text{O}$.
- 5 Locate the Reaction Rate section. From the list, choose User defined.

- 6 In the r_j text field, type $\text{re.kf_2}*\text{re.c_NO2}*\text{re.c_NO}*\text{re.c_NH3}/(1+\text{K_NH3}*\text{re.c_NH3})$.
- 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) NO2 SCR: $8 \text{ NH}_3 + 6 \text{ NO}_2 \Rightarrow 7 \text{ N}_2 + 12 \text{ H}_2\text{O}$

- 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 $8 \text{ NH}_3 + 6 \text{ NO}_2 \Rightarrow 7 \text{ N}_2 + 12 \text{ H}_2\text{O}$.
- 4 In the Label text field, type (3) NO2 SCR: $8 \text{ NH}_3 + 6 \text{ NO}_2 \Rightarrow 7 \text{ N}_2 + 12 \text{ H}_2\text{O}$.
- 5 Locate the Reaction Rate section. From the list, choose User defined.
- 6 In the r_j text field, type $\text{re.kf_3}*\text{re.c_NO2}*\text{re.c_NH3}/(1+\text{K_NH3}*\text{re.c_NH3})$.
- 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: $2 \text{ NO} + \text{O}_2 \rightleftharpoons 2 \text{ NO}_2$

- 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 $2 \text{ NO} + \text{O}_2 \rightleftharpoons 2 \text{ NO}_2$.
- 4 Click Apply.
- 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.

▼ Rate Constants

☒ Specify equilibrium constant

☒ Use Arrhenius expressions

$$k^f = A^f (T/T_{\text{ref}})^{n^f} \exp\left(\frac{-E^f}{R_g T}\right), T_{\text{ref}} = 1\text{K}$$

$$k^r = k^f/K_j$$

Forward frequency factor:

A^f $\text{m}^3/(\text{s}\cdot\text{mol}^2)$

Forward temperature exponent:

n^f 1

Forward activation energy:

E^f J/mol

- 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.

- 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:

The screenshot shows the 'Mixture Properties' section with the 'Thermodynamics' checkbox checked. The 'Thermodynamic system' is set to 'Gas System 1', the 'Phase' is 'Gas', and the 'Reactor pressure' is 'User defined' at 1 [atm]. Below this is the 'Species Matching' table:

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

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.

- 13 In the Model Builder window, under Component 1 > Reaction Engineering click 4: 2 NO + O2 <=> 2 NO2.

- 14 In the Settings window for Reaction, type (4) Equilibrium: NO + O2 <=> 2 NO2 in the Label text field.

(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 $4 \text{ NH}_3 + 3 \text{ O}_2 \Rightarrow 2 \text{ N}_2 + 6 \text{ H}_2\text{O}$.
- 4 In the Label text field, type (5) Undesired 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 $\text{re.kf_5} * (\text{re.c_NH}_3 * \text{re.c_O}_2) / (1 + \text{K_NH}_3 * \text{re.c_NH}_3)$.
- 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) UNDESIED NO FORMATION: $4 \text{ NH}_3 + 5 \text{ O}_2 \Rightarrow 4 \text{ NO} + 6 \text{ H}_2\text{O}$

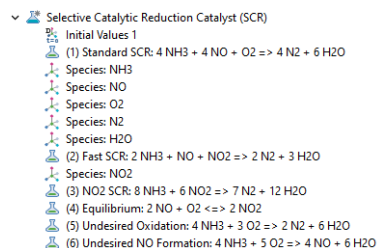
- 1 In the Reaction Engineering toolbar, click  Reaction.
- 2 In the Settings window for Reaction, locate the Reaction Formula section.
- 3 In the Formula text field, type $4 \text{ NH}_3 + 5 \text{ O}_2 \Rightarrow 4 \text{ NO} + 6 \text{ H}_2\text{O}$.
- 4 In the Label text field, type (6) Undesied 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 $\text{re.kf_6} * \text{re.c_O}_2 * \text{re.c_NH}_3 / G$.
- 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 rename the interface to something descriptive.

- 11 In the Model Builder window, click Reaction Engineering.

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

After setting up the reaction kinetics, define the suitable reactor model where the reactions take place. Using the Reaction Engineering node you can choose one of the predefined reactor types.



Since you are planning to set up a single channel model, having chosen the Stationary Plug Flow study type previously, choose the Plug flow reactor.

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 1.
- 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	FH20_in
N2	FN2_in
NH3	FNH3_in
NO	FNO_in
NO2	FN02_in
O2	F02_in

Now that the reactions and kinetics settings are set, use Equation View to check what variable names were generated. These variable names should be those used in the imported variable definitions under the Definitions node.

Equation View

- 1** In the Model Builder window, click Show More Options .
- 2** Under Physics, check Equation View  checkbox. Click OK.
- 3** In the Model Builder window, expand the (1) Standard SCR: $4 \text{ NH}_3 + 4 \text{ NO} + \text{O}_2 \Rightarrow 4 \text{ N}_2 + 6 \text{ H}_2\text{O}$ node . Click Equation View. Scroll through the Variables list to see the generated variable names, expressions, units, and descriptions.

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

Variables

Name	Expression	Unit	Description
re.Qheat	-re.r_1*re.H_1	W/m³	Heat source of reactions
re.Tref_1	1[K]	K	Reference temperature
re.Af_1	A1_SCR	m³/(s·mol²)	Forward frequency factor
re.nf_1	0	1	Forward temperature exponent
re.Ef_1	E1_SCR	J/mol	Forward activation energy
re.kf_1	re.Af_1*(re.T/re.Tref_1)...	m³/(s·mol²)	Forward rate constant
re.r_1	re.kf_1*re.c_NO*re.c_O...	mol/(m³·s)	Reaction rate
re.R_NH3	-4*re.r_1	mol/(m³·s)	Reaction rate for species NH3

Reaction Kinetics for the Ammonia Slip Catalyst (ASC)

- 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.
- 4 Click the Add to Component 1 button in the window toolbar.
- 5 In the Home toolbar, click  Add Physics to close the Add Physics window.
- 6 In the Settings window for Reaction Engineering, type Ammonia Slip Catalyst (ASC) in the Label text field.
- 7 Locate the Reactor section. From the Reactor type list, choose Plug flow.
- 8 Locate the Energy Balance section. From the Energy balance list, choose Include.

Add the reactions.

(1) DESIRED NH3 OXIDATION: $4 \text{ NH}_3 + 3 \text{ O}_2 \Rightarrow 2 \text{ N}_2 + 6 \text{ H}_2\text{O}$

- 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 $\text{re}2.\text{kf}_1*\text{re}2.\text{c_NH}_3*\text{re}2.\text{c_O}_2/(1+\text{K_NH}_3_\text{ASC}*\text{re}2.\text{c_NH}_3)$.
- 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) UNDESIRE NO FORMATION: $4 \text{ NH}_3 + 5 \text{ O}_2 \Rightarrow 4 \text{ NO} + 6 \text{ H}_2\text{O}$

- 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 $\text{re2.kf_2*re2.c_O2*re2.c_NH3/G_ASC}$.
- 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: $2 \text{ NO} + \text{O}_2 \rightleftharpoons 2 \text{ NO}_2$

- 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 $2 \text{ NO} + \text{O}_2 \rightleftharpoons 2 \text{ NO}_2$.
- 4 In the Label text field, type (3) Equilibrium: $2 \text{ NO} + \text{O}_2 \rightleftharpoons 2 \text{ NO}_2$.
- 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) UNDESIRE NO2 FORMATION: $4 \text{ NH}_3 + 7 \text{ O}_2 \Rightarrow 4 \text{ NO}_2 + 6 \text{ H}_2\text{O}$

- 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 $4 \text{ NH}_3 + 7 \text{ O}_2 \Rightarrow 4 \text{ NO}_2 + 6 \text{ H}_2\text{O}$.
- 4 In the Label text field, type (4) Undesired NO2 formation: $4 \text{ NH}_3 + 7 \text{ O}_2 \Rightarrow 4 \text{ NO}_2 + 6 \text{ H}_2\text{O}$.

- 5 Locate the Reaction Rate section. From the list, choose User defined.
- 6 In the r_j text field, type $re2.kf_4*re2.c_NH3*re2.c_O2/G_ASC$.
- 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).
- 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.

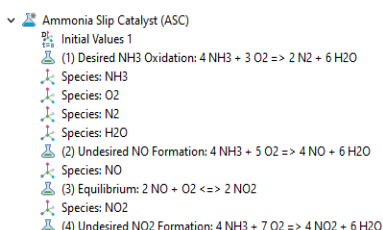
INITIAL VALUES I

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

The ammonia slip catalyst interface now looks like this:



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 1: SCR Operating Window, Fixed ANR

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 v_SCR.
- 4 Locate the Physics and Variables Selection section. In the Solve for column of the table, under Component 1, clear the checkbox for Ammonia Slip Catalyst (ASC).

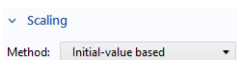
- Click to expand the Study Extensions section. Select the Auxiliary sweep checkbox.
- Click  Add.
- In the table, enter the following settings:

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.

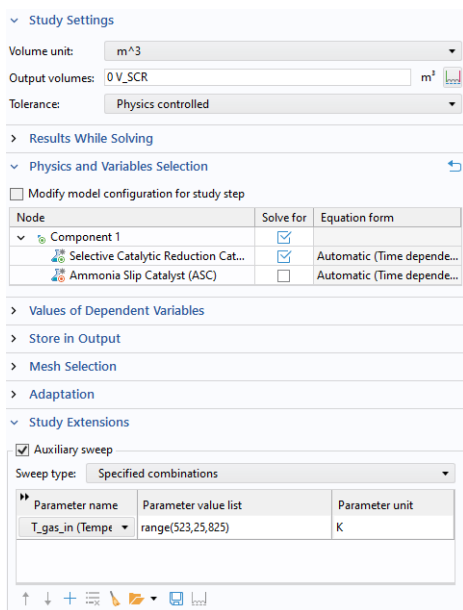
SOLUTION 1 (sol1)

- In the Study toolbar, click  Show Default Solver.
- In the Model Builder window, expand the Solution 1 (sol1) node, then click Dependent Variables 1.
- In the Settings window for Dependent Variables, locate the Scaling section.
- From the Method list, choose Initial-value based.



Rename the study into something descriptive, and compute.

- In the Model Builder window, click Study 1.
- In the Settings window for Study, type Study 1: SCR Temperature Operating Window, ANR = 1.3, Case 2 in the Label text field.
- In the Study toolbar, click  Compute.



Results for Study I

Take a look at the resulting default plots. Modify them and follow the below steps to create [Figure 3](#), [Figure 4](#), and [Figure 5](#).

FIGURE 3: CONVERSION ALONG REACTOR AXIS

- 1 In the Settings window for 1D 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.
- 4 In the Model Builder window, expand the Conversion Along Reactor Axis node, then click Global 1.
- 5 In the Settings window for Global, locate the y-Axis Data section.
- 6 Click  Clear Table.
- 7 In the table, enter the following settings:

EXPRESSION	UNIT	DESCRIPTION
X_NOx_SCR	1	NOx Conversion in SCR

- 8 Click to expand the Coloring and Style section. From the Color cycle list, choose Long.
- 9 From the Width list, chose 2.
- 10 Find the Line markers subsection. From the Marker list, choose Cycle.
- 11 In the Number text field, type 1.
- 12 Click to expand the Legends section. Find the Include subsection. Clear the Expression checkbox.
- 13 Click the  Zoom Extents button in the Graphics toolbar.
- 14 In the Conversion Along Reactor Axis toolbar, click  Plot.

The plot in [Figure 3](#) has now been set up. Duplicate this plot group to use as a basis for setting up [Figure 4](#).

FIGURE 4: 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 1D Plot Group, type Temperature Increase Along Reactor Axis in the Label text field.

- 4 In the Model Builder window, expand the Conversion Along Reactor Axis node, then click Global I
- 5 In the Settings window for Global, locate the y-Axis Data section.
- 6 In the table, enter the following settings:

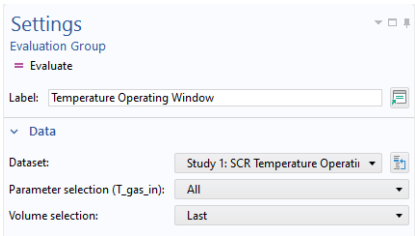
EXPRESSION	UNIT	DESCRIPTION
re.T-T_gas_in	K	Temperature Increase

- 7 Click the  Zoom Extents button in the Graphics toolbar.
- 8 In the Temperature Increase Along Reactor Axis toolbar, click  Plot.

By using an Evaluation Group we can create a table containing the final conversion values for each run in the Parametric Sweep study. That table can then be plotted to give [Figure 5](#). That is what we will do next.

FIGURE 5: 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.



- 4 Right-click Temperature Operating Window and choose Global Evaluation.
- 5 In the Settings window for Global Evaluation, locate the Expressions section.
- 6 Click  Clear Table.
- 7 In the table, enter the following settings:

EXPRESSION	UNIT	DESCRIPTION
X_NOx_SCR	1	NOx Conversion in SCR

- 8 In the Temperature Operating Window toolbar, click  Evaluate.

9 Go to the Temperature Operating Window. It contains the data from the Evaluation.

10 Click the  Table Graph button in the window toolbar.

11 In the Settings window for Table Graph, locate the Data section.

12 From the Plot columns list, choose Manual.

13 In the Columns list, select NOx Conversion in SCR (1).

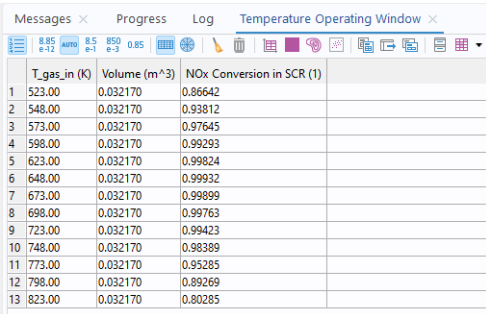
14 Locate the Coloring and Style section. From the Width list, choose 2.

15 In the Model Builder window, under Results click 1D Plot Group 3.

16 In the Settings window for 1D Plot Group, type Temperature Operating Window in the Label text field.

17 Click the  Zoom Extents button in the Graphics toolbar.

18 In the Temperature Operating Window toolbar, click  Plot.



	T_gas_in (K)	Volume (m ³)	NOx Conversion in SCR (1)
1	523.00	0.032170	0.86642
2	548.00	0.032170	0.93812
3	573.00	0.032170	0.97645
4	598.00	0.032170	0.99293
5	623.00	0.032170	0.99824
6	648.00	0.032170	0.99932
7	673.00	0.032170	0.99899
8	698.00	0.032170	0.99763
9	723.00	0.032170	0.99423
10	748.00	0.032170	0.98389
11	773.00	0.032170	0.95285
12	798.00	0.032170	0.89269
13	823.00	0.032170	0.80285

SCR TEMPERATURE OPERATING WINDOW, ANR = 1.3, CASE 2

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

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.

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

4 As a final cleaning-up action, in the Model Builder window, right-click Temperature (re) and choose Delete.

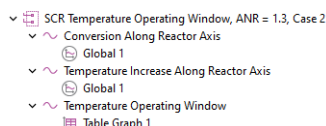
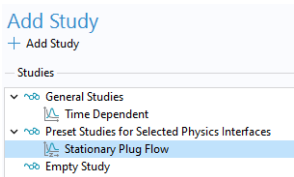


Figure 3, Figure 4, and Figure 5 are now done. Continue by investigating the SCR operation as a function of both inlet temperature and ammonia to NOx ratio (ANR). Such a study will generate a lot of data due to the many parameter combinations. Therefore, turn off generate default plots, choose Only plot 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.



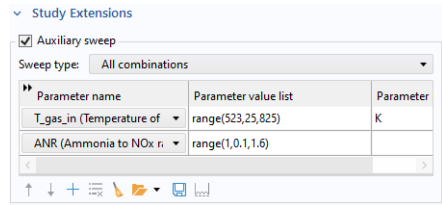
Study 2: SCR Operating Window, Effect of ANR

We will reuse the work we spent on setting up Study 1. Therefore, delete the default study step in Study 2, and copy paste the study steps used in Study 1.

- 1 In the Model Builder window, under Study 2 right-click
Step 1: Stationary Plug Flow and choose Delete.
- 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.
- 3 In the Model Builder window, right-click Study 2 and choose
Paste Stationary Plug Flow.
- 4 In the Settings window for Stationary Plug Flow, locate the Study Extensions
section.
- 5 Click  Add.
- 6 In the table, enter the following settings:

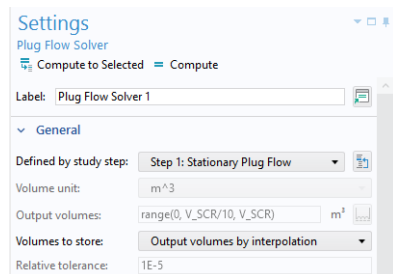
PARAMETER NAME	PARAMETER VALUE LIST	PARAMETER UNIT
ANR (Ammonia to NOx ratio in gas entering the reactor)	range(1,0.1,1.6)	

- 7 From the Sweep type list, choose All combinations.
- 8 Locate the Study Settings section. In the Output volumes text field, type $\text{range}(0, V_{\text{SCR}}/10, V_{\text{SCR}})$.
- 9 In the Model Builder window, click Study 2.
- 10 In the Settings window for Study, locate the Study Settings section.
- 11 Clear the Generate default plots checkbox.
- 12 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.
- 8 In the Model Builder window, click Results.
- 9 In the Settings window for Results, locate the Update of Results section.
- 10 Select the Only plot when requested checkbox.
- 11 In the Study toolbar, click Compute.

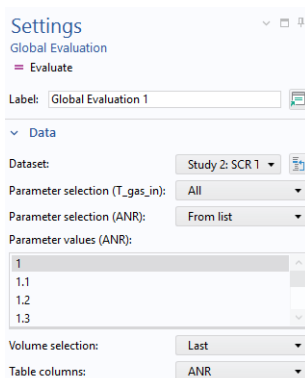


Results for Study 2

Reuse our previous work spent on setting up the Evaluation Group for [Figure 3](#) by duplicating this group in order to generate [Figure 6](#).

EVALUATION GROUP FOR FIGURE 6

- 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.
- 4 In the Model Builder window, expand the Temperature Operating Window and ANR Effect, NO_x Conversion node, then click Global Evaluation 1.
- 5 In the Settings window for Global Evaluation, locate the Data section.
- 6 From the Dataset list, choose Study 2: SCR Temperature Operating Window, ANR Effect, Case 2/Solution 2 (sol2).
- 7 From the Parameter selection (ANR) list, choose From list.
- 8 In the Parameter values (ANR) list, select 1.
- 9 From the Volume selection list, choose Last.
- 10 From the Table columns list, choose ANR.



Global Evaluation 2

- 1 Right-click Results > Temperature Operating Window and ANR Effect, NO_x 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, select 1.1.

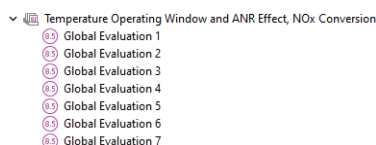
Global Evaluation 3

- 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, 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, select 1.3.

Continue with these three steps until you have added seven Global Evaluation Groups and thus created data for ANR values from 1 to 1.6.



- 4 In the Model Builder window, click Temperature Operating Window and ANR Effect, NOx Conversion.
- 5 In the Temperature Operating Window and ANR Effect, NOx Conversion toolbar, click Evaluate.

FIGURE 6: NOX CONVERSION IN SCR

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

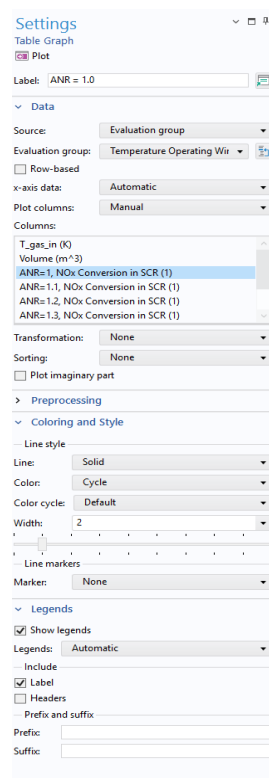
ANR = 1.0

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

- 8 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, 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, select $ANR=1.2$, NO_x Conversion in SCR (1).

Repeat these three steps until there are seven Table Graph nodes, from $ANR 1.0$ to $ANR 1.6$.

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

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

EVALUATION GROUP FOR FIGURE 7

- 1 In the Model Builder window, right-click Temperature Operating Window and ANR Effect, NO_x Conversion and choose Duplicate.
- 2 In the Model Builder window, click Temperature Operating Window and ANR Effect, NO_x Conversion 1.
- 3 In the Settings window for Evaluation Group, type Temperature Operating Window and ANR Effect, NH_3 Conversion in the Label text field.
- 4 In the Settings window for 1D Plot Group, locate the Legend section.
- 5 From the Position list, choose Lower right.
- 6 In the Model Builder window, click Global Evaluation 1.
- 7 In the Settings window for Global Evaluation, locate the Expressions section.

8 In the table, enter the following settings:

EXPRESSION	UNIT	DESCRIPTION
X_NH3_SCR	1	NH3 Conversion in SCR

9 In the same way, edit the Expression for the other Global Evaluations in this Evaluation Group.

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

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

FIGURE 7: 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 1D 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.

7 In the Model Builder window, click ANR = 1.0.

8 In the Settings window for Table Graph, locate the Data section.

9 From the Evaluation group list, choose Temperature Operating Window and ANR Effect, NH3 Conversion.

10 Repeat the previous step for each of the remaining Table Graphs in the Plot Group.

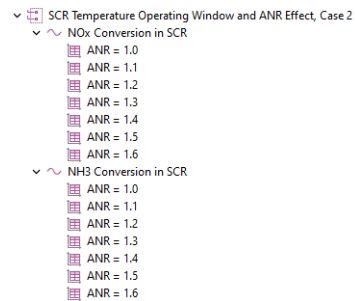
11 Click the  Zoom Extents button in the Graphics toolbar.

12 In the NH3 Conversion in SCR toolbar, click  Plot.

SCR TEMPERATURE OPERATING WINDOW AND ANR EFFECT, CASE 2

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

- 1 In the Model Builder window, under Results, Ctrl-click to select NO_x Conversion in SCR and NH₃ Conversion in SCR.
- 2 Right-click and choose Group.
- 3 In the Settings window for Group, type SCR Temperature Operating Window and ANR Effect, Case 2 in the Label text field.



Study 3: Single Channel Model, Effect of ANR

We have now investigated the influence of both inlet temperature and ammonia to NO_x 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.

- 1 In the Model Builder window, click Results.
- 2 In the Settings window for Results, locate the Update of Results section.
- 3 Clear the Only plot when requested checkbox.
- 4 In the Home toolbar, click  Add Study to open the Add Study window.
- 5 Go to the Add Study window.
- 6 Find the Studies subsection. In the Select Study tree, select Preset Studies for Selected Physics Interfaces > Stationary Plug Flow.
- 7 Click the Add Study button in the window toolbar.
- 8 In the Home toolbar, click  Add Study to close the Add Study window.

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, clear the checkbox for Ammonia Slip Catalyst (ASC).

STATIONARY PLUG FLOW, ASC

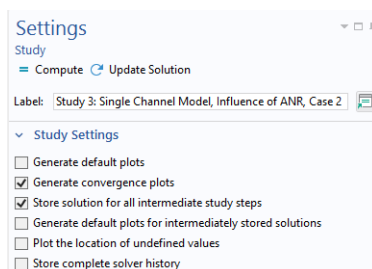
- 1 Right-click Study 3 > Step 1: Stationary Plug Flow, SCR and choose Duplicate.
- 2 In the Settings window for Stationary Plug Flow, type Stationary Plug Flow, ASC in the Label text field.
- 3 Locate the Study Settings section. In the Output volumes text field, type $V_SCR + V_ASC$.
- 4 Locate the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

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  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.

SOLVER CONFIGURATIONS

Use initial value based scales for the dependent variables.

1 In the Model Builder window, expand the

Study 3: Single Channel Model, Influence of ANR, Case 2 > Solver Configurations node.

2 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.

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, 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.

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.

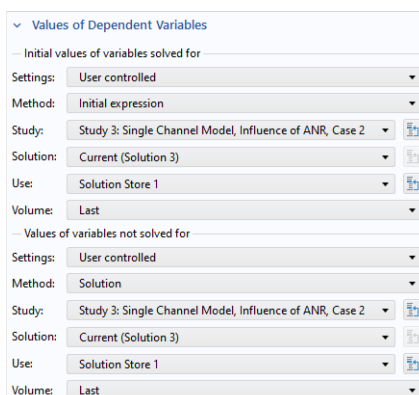
2 In the Settings window for Parametric Sweep, locate the Study Settings section.

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.



Results for Study 3

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

FIGURE 8: MOLAR FRACTION OF NH3 AND NOX

- 1 In the Results toolbar, click  1D Plot Group.
- 2 In the Settings window for 1D Plot Group, type Molar Fraction of NH3 and NOx 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 NOx 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 > 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 NH₃.

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
yNO _x _SCR	ppm	Molar fraction of NO _x 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 1 (sol5).
- 4 Locate the y-Axis Data section. In the table, enter the following settings:

EXPRESSION	UNIT	DESCRIPTION
yNO _x _ASC	ppm	Molar fraction of NO _x 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 1D 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 $\text{Reactor volume (m}^3\text{)}$.
- 6 Select the y-axis label checkbox. In the associated text field, type $\text{Molar Fraction of NH}_3\text{ (ppm)}$.
- 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 $\text{Molar Fraction of NOx (ppm)}$.
- 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 9](#).

FIGURE 9: 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 1.
- 3 In the Settings window for 1D 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 1 > Definitions > Variables > X_NH3_SCR - NH3 Conversion in SCR - 1.

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

NOx SCR

- 1 In the Model Builder window, click NOx 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

NOx

- 1 In the Model Builder window, click NOx.
- 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 NOx 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. But first, add the last two plots in a Group with a suitable name.

SINGLE CHANNEL MODEL, INFLUENCE OF ANR, CASE 2

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

Study 4: Single Channel Model, Influence of Engine Load

Just like with previous studies, to save time, reuse the study groups already set-up.

- 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.
- 6 In the Settings window for Study, type Study 4: Single Channel Model, ANR = 1.3, All Cases in the Label text field.
- 7 Clear the Generate default plots checkbox.
- 8 Locate the Study Settings section. Select the Store solution for all intermediate study steps checkbox.
- 9 In the Model Builder window, under Study 4: Single Channel Model, Influence of ANR, All Cases, right-click Step 1: Stationary Plug Flow and choose Delete.
- 10 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.
- 11 Right-click and choose Copy.
- 12 In the Model Builder window, right-click Study 4: Single Channel Model, Influence of ANR, All Cases and choose Paste Multiple Items.

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.

Results for Study 4

The following steps generate [Figure 10](#) and [Figure 11](#).

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.

FIGURE 10: 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 1D 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.

FIGURE 11: 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 1D 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 12](#).

FIGURE 12: 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 1D Plot Group, type Temperature Increase Along Reactor Axis, All Cases in the Label text field.
- 3 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, Influence of ANR, Case 2 > 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, Influence of ANR, Case 2 > 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, Influence of ANR, Case 2 > 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

- 8 In the Model Builder window, click Temperature Increase Along Reactor Axis, All Cases.
- 9 In the Settings window for 1D Plot Group, locate the Legend section.
- 10 In the Number of columns text field, type 3.
- 11 In the Maximum relative width text field, type 1.
- 12 Click the  Zoom Extents button in the Graphics toolbar.
- 13 In the Temperature Increase Along Reactor Axis, All Cases toolbar, click  Plot.

SINGLE CHANNEL MODEL

- 1 In the Model Builder click Component 1.
- 2 Type Single Channel Model in the Label text field.

Preparing to Model the Full Monolith Reactor

In the next phase of this example, set up a space-dependent 2D axisymmetric model of the monolithic reactor, including mass transport and reaction, heat transfer, and fluid flow.

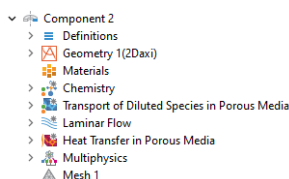
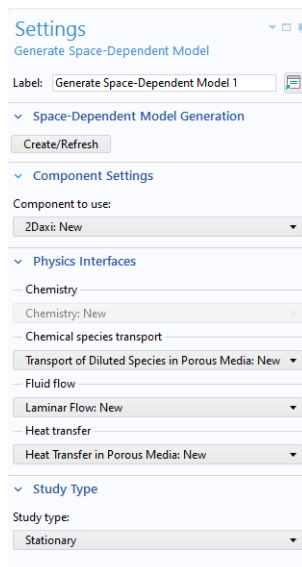
The Monolith Reactor Model uses the plug flow Single Channel Model as a base. The Generate Space-Dependent Model feature creates a link between the plug flow reactor model and the space-dependent monolith model. It allows you to transfer reaction kinetics, thermodynamics, and transport properties set up in the Reaction Engineering interfaces to the physics interfaces describing space and time-dependent systems.

GENERATE SPACE-DEPENDENT MODEL

- 1 In the Model Builder window, under Single Channel Model click Selective Catalytic Reduction Catalyst (SCR).
- 2 In the Reaction Engineering toolbar click Generate Space-Dependent Model  (or right-click Reaction Engineering  and choose it from the menu).

- 3 In the Settings window for Generate Space-Dependent Model, locate the Component Settings section. Choose 2Daxi: New from the Component to use list.
- 4 Locate the Physics Interfaces section. Find the Chemical species transport subsection. From the list, choose Transport of Diluted Species in Porous Media: New.
- 5 Find the Fluid flow subsection. From the list, choose Laminar Flow: New.
- 6 Find the Heat transfer subsection. From the list, choose Heat Transfer in Porous Media: New.
- 7 Locate the Space-Dependent Model Generation section. Click Create/Refresh. A 2Daxi Component is created.

The new 2Daxi component, called Component 2, appears in the Model Builder window. A Chemistry node is automatically created for the SCR. It includes the kinetic, thermal, and transport properties setup in the Reaction Engineering interface that it was generated from. If necessary, changes can be made directly to this node.



Note: In addition to the physics interfaces that were added with the Generate Space-Dependent Model feature, additional interfaces can be added by clicking Add Physics  in the Home toolbar.

Modeling Instructions: Monolith Reactor Model

First, rename the Component node.

- 1 In the Model Builder click Component 2.
- 2 Type Monolith Reactor Model in the Label text field.

GEOMETRY

Now import a file with the reactor geometry. Symmetry reduces the modeling domain.

- 1 In the Model Builder window, expand the Monolith Reactor Model node.
- 2 Right-click Monolith Reactor Model > Geometry 1(2Daxi) and choose Insert Sequence .
- 3 Browse to the model's Application Libraries folder and double-click the file monolith_reactor_geom_sequence.mph.

Note: The location of a file is based on the installation. For example, if the installation is on your hard drive, the file path might be similar to C:\Program Files\COMSOL\COMSOL64\Multiphysics\applications\.

- 4 In the Geometry toolbar, click  Build All.

Note: In this step-by-step, focusing on the Chemical Reaction Engineering Module, all geometry settings are already done. For information, a central part of the model setup consists of assigning features to domains and boundaries of the model geometry. The use of Explicit Selections  features added to the geometry makes this process more efficient. The imported geometry sequence contains eight predefined Explicit Selection nodes. The names and the selected entities of these selections are seen in the table below.

NODE NAME	DOMAINS OR BOUNDARIES SELECTED
SCR Catalyst	domain 5
ASC Catalyst	domain 3
Mat Domain	domain 14
Metal Shell Domain	domain 7, 15
Flow Inlet	boundary 12
Flow Outlet	boundary 6
Free Flow Domain	domain 4
Insulating Gas	domain 8-13, 16-18

Domains or boundaries can be assigned to the Explicit nodes by clicking in the geometry. This adds the identification number of the domain or boundary to the Input Entities list. To remove a selection, click again to toggle.

Apart from Explicit Selections , it is also possible to add Union Selection . Such selections combine one or more Explicit Selections. This is shown later in section [Union Selections](#) in this modeling instructions.

Explicit Selections, Union Selections, and a range of other Selection nodes are available from the Selections  menu in the Geometry toolbar.

PARAMETERS

Parameters: Temperature and Monolith Parameters

- 1 In the Model Builder window, under Global Definitions click Parameters: Temperature and Monolith Parameters.
- 2 In the Settings window for Parameters, locate the Parameters section.
- 3 Click Click  Load from File.
- 4 Browse to the model's Application Libraries folder and double-click the file `monolith_reactor_temperature_monolith_parameters.txt`.

VARIABLES

Moving on by loading variables from file. The variables in the variable expressions have not yet been created and this is indicated with yellow text in the expression fields. We load the variables from file for convenience, but the variables can also be added manually.

Variables: SCR Kinetics

- 1 In the Home toolbar, click Variables  and choose Local variables. Optionally, go to the Model Builder window, expand the Monolith Reactor Model, right-click Definitions , and choose Variables .
- 2 In the Settings window for Variables, locate the Geometric Entity Selection section.
- 3 From the Geometric entity level list, choose Domain.
- 4 From the Selection list, choose SCR Catalyst.
- 5 Locate the Variables section. Click  Load from File.
- 6 Browse to the model's Application Libraries folder and double-click the file `monolith_reactor_SCR_kinetics_variables.txt`.
- 7 In the Label text field, type Variables: SCR Kinetics.

Variables: ASC Kinetics

- 1 Right-click Definitions and choose Variables.
- 2 In the Settings window for Variables, type Variables: ASC Kinetics in the Label text field.
- 3 Locate the Geometric Entity Selection section. From the Geometric entity level list, choose Domain.
- 4 From the Selection list, choose ASC Catalyst.
- 5 Locate the Variables section. Click  Load from File.
- 6 Browse to the model's Application Libraries folder and double-click the file `monolith_reactor_ASC_kinetics_variables.txt`.

Variables: Postprocessing

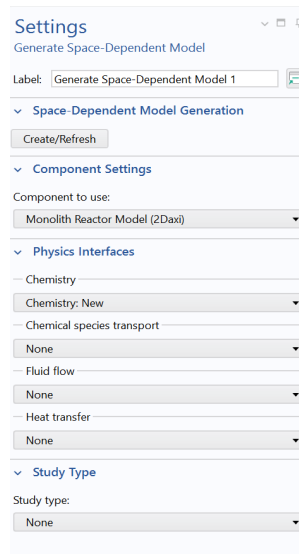
- 1 Right-click Definitions and choose Variables.
- 2 In the Settings window for Variables, type Variables: Postprocessing in the Label text field.
- 3 Locate the Variables section. Click  Load from File.
- 4 Browse to the model's Application Libraries folder and double-click the file `monolith_reactor_postprocessing_variables.txt`.

GENERATE SPACE-DEPENDENT MODEL FOR THE AMMONIA SLIP CATALYST

The Chemistry interface in the 2Daxi component contains the SCR chemistry. Generate a Chemistry interface for the ammonia slip catalyst by using the Generate Space-Dependent Model functionality.

In the Model Builder window, under Single Channel Model click Ammonia Slip Catalyst (ASC).

- 1 In the Reaction Engineering toolbar, click  Generate Space-Dependent Model.
- 2 In the Settings window for Generate Space-Dependent Model, locate the Component Settings section.
- 3 From the Component to use list, choose Monolith Reactor Model.
- 4 Locate the Physics Interfaces section. Find the Chemical species transport subsection. From the list, choose None.
- 5 Find the Fluid flow subsection. From the list, choose None.



- 6 Find the Heat transfer subsection. From the list, choose None.
- 7 Locate the Study Type section. From the Study type list, choose None.
- 8 Locate the Space-Dependent Model Generation section. Click Create/Refresh.
- 9 In the Model Builder window, under Monolith Reactor Model click Chemistry 2.
- 10 In the Settings window for Chemistry, type Chemistry: ASC in the Label text field.

Materials

The next step is to specify material properties for the model. Ready-to-use materials can be selected from the available libraries or generated from Thermodynamics. In this model, first generate a material node for nitrogen (solvent) from our Gas System, under Thermodynamics. After that, generate the solid monolith material. Both these materials are then used to create a Porous Material.

The created materials are assigned to the relevant selections in the geometry. This allows the physics interfaces in these selections to access the material properties.

GENERATE MATERIAL

- 1 In the Model Builder, under Global Definitions , locate Thermodynamics  > Gas System .
- 2 Right-click on Gas System and choose Generate Material .
This opens the Generate Material wizard which consists of several steps to create a Material node from our property package.
- 3 In Select Phase window, choose Gas (default) and click Next .
- 4 All species in the system has been added to the Select species table by default.
- 5 In the Material composition section, click the mass fraction button
- 6 Use the table to set mass fraction of nitrogen as 1 and 0 for others.
- 7 Click Next  in the wizard.

- 8 In the Select Properties window, choose Diffusion coefficient at infinite dilution, and click Add Selected + .
- 9 In the Select solvent subsection, choose nitrogen in the list of species. Click Next → .
- 10 In the Define Material window, choose Global from the Component list. This adds the material to the global Material node and thus makes it accessible in any component in the model.
- 11 From the Function type list, choose Interpolation. This creates fast to evaluate interpolation functions for the material properties.
- 12 Set the Temperature upper bound (High) to 733.
- 13 Click Finish ☒ to create the material.

Generate Material Wizard ▾ □

Select Properties

Back Next Finish

Amount base unit:

kg

Type filter text

Density (kg/m³)

Diffusion coefficient at infinite dilution (m²/s)

Heat capacity (Cp) (J/(K*kg))

Heat capacity ratio (Cp/Cv)

Thermal conductivity (W/(m*K))

Viscosity (Pa*s)

+

Selected properties:

Name	Unit
Density (kg/m ³)	kg/m ³
Heat capacity (Cp) (J/(K*kg))	J/kg/K
Heat capacity ratio (Cp/Cv)	1
Thermal conductivity (W/(m*K))	W/m/K

GAS: NITROGEN SOLVENT

- 1 In the Model Builder, expand the Global Definitions > Materials node, and select the created material node where the composition is indicated:
Gas: ammonia(0)-nitrogen(1)-nitrogen oxide(0)-oxygen(0)- water(0) .
- 2 In the Settings window, change the Label to Gas: Nitrogen Solvent, to use a simpler name.

Next, create a user-defined material and associate it with the solid monolith material.

SOLID: MONOLITH MATERIAL

- 1 In the Materials toolbar, click Blank Material .
- 2 In the Model Builder window, expand the Material 1 node, then click Basic.
- 3 In the Settings window, locate the Output Properties section. Click Select Quantity + below the table.
- 4 In the Physical Quantity dialog, type density in the text field and click Filter . Select Density (kg/m³). Click OK.

Settings ▾ □

Basic

Label: Basic

Name: def

Output Properties

Property	Variable	Expression	Unit	Size	Info
Density	rho	2970[kg/m ³]	kg/m ³	1x1	
Heat capacity at constant pressure	Cp	975[J/kg/K]	J/(kg*K)	1x1	
Thermal conductivity	k_iso ; kii =...	35[W/m/K]	W/(m*K)	3x3	

- 5 Perform the same action for the properties heat capacity (choose Heat capacity at constant pressure (J/(kg·K)) and thermal conductivity (choose Thermal conductivity (W/(m·K))).
- 6 Add expressions to the Output Properties section. Type 2970[kg/m³] for the density, 975[J/kg/K] for the heat capacity, and 35[W/m/K] for the thermal conductivity.
- 7 In the Model Builder window, select the Material 1 and type Solid: Monolith Material in the Label field to name it accordingly.

In the next stage of the modeling process, add a Porous Material that consists of the two materials that were just defined.

POROUS MATERIAL

- 1 In the Materials toolbar, click More Materials and choose Local > Porous Material .
- 2 In the Settings window for Porous Material, locate the Geometric Entity Selection section. From the Selection list, choose Domains 3, 5, and 14.

FLUID

- 3 Right-click Porous Material and choose Fluid  from the context menu. Notice that the generated global material Gas: Nitrogen Solvent is predefined for this node.
- 4 Right-click Porous Material and choose Solid  from the context menu.
- 5 In the Solid Properties section, choose Solid: Monolith Material in the Material list.
- 6 In the Volume fraction θ_s text field, type 1-por.

Add a material for the metal parts of the reactor.

METAL

- 1 In the Home toolbar, click  Windows and choose Add Material from Library.
- 2 Go to the Add Material window.
- 3 In the tree, select Built-in > Structural steel.
- 4 Click the Add to Component button in the window toolbar.
- 5 In the Settings window for Material, locate the Geometric Entity Selection section.
- 6 From the Selection list, choose Metal Shell Domain.

Note: A description of how to set up these selections can be found in [Geometry](#).

Add a material for the insulating air in the reactor wall.

AIR

- 1 In the Home toolbar, click  Windows and choose Add Material from Library.
- 2 Go to the Add Material window.
- 3 In the tree, select Built-in > Air.
- 4 Click the Add to Component button in the window toolbar.
- 5 In the Home toolbar, click  Add Material to close the Add Material window.
- 6 In the Settings window for Material, locate the Geometric Entity Selection section.
- 7 From the Selection list, choose Insulating Gas.

Add a Material Link to the nitrogen gas to create a material for the free flowing gas between the two catalysts.

FREE FLOW DOMAIN MATERIAL

- 1 In the Model Builder window, right-click Materials and choose More Materials > Material Link.
- 2 In the Settings window for Material Link, locate the Geometric Entity Selection section.
- 3 From the Selection list, choose Free Flow Domain.
- 4 In the Label text field, type Free Flow Domain Material.

Complete the settings for the two Chemistry interfaces by setting the concentration of nitrogen and coupling the ammonia slip catalyst chemistry to the mass transfer interface.

Chemistry: SCR

- 1 In the Model Builder window, under Monolith Reactor Model click Chemistry.
- 2 In the Settings window for Chemistry, type Chemistry: SCR in the Label text field.
- 3 Locate the Species Matching section.

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

SPECIES	TYPE	MOLAR CONCENTRATION	VALUE (MOL/M^3)	FROM THERMODYNAMICS
H2O	Variable	cH2O	Solved for	H2O
N2	Solvent	User defined	cN2_in	N2
NH3	Variable	cNH3	Solved for	H3N
NO	Variable	cNO	Solved for	NO
NO2	Variable	cNO2	Solved for	NO2
O2	Variable	cO2	Solved for	O2

Chemistry: ASC

- 1 In the Model Builder window, under Monolith Reactor Model click Chemistry: ASC.
- 2 In the Settings window for Chemistry, locate the Species Matching section.
- 3 Find the Bulk species subsection. From the Species solved for list, choose Transport of Diluted Species in Porous Media.
- 4 In the table, enter the following settings:

SPECIES	TYPE	MOLAR CONCENTRATION	VALUE (MOL/M^3)	FROM THERMODYNAMICS
H2O	Variable	cH2O	Solved for	H2O
N2	Solvent	User defined	cN2_in	N2
NH3	Variable	cNH3	Solved for	H3N
NO	Variable	cNO	Solved for	NO
NO2	Variable	cNO2	Solved for	NO2
O2	Variable	cO2	Solved for	O2

Before setting up the heat, mass, and momentum physics, add selections that can be used for these physics interfaces.

Union Selections

POROUS AND FREE FLOW DOMAINS

- 1 In the Geometry toolbar, click  Selections and choose Union Selection.
- 2 In the Settings window for Union Selection, type Porous and Free Flow Domains in the Label text field.
- 3 Locate the Input Entities section. Click  Add.
- 4 In the Add dialog, in the Selections to add list, choose SCR Catalyst, ASC Catalyst, and Free Flow Domain.
- 5 Click OK.

HEAT TRANSFER DOMAINS

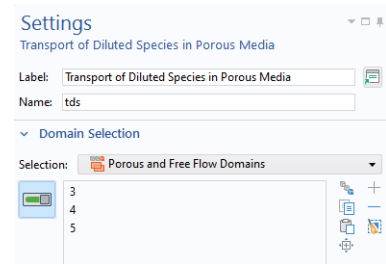
- 1 In the Geometry toolbar, click  Selections and choose Union Selection.
- 2 In the Settings window for Union Selection, type Heat Transfer Domains in the Label text field.
- 3 Locate the Input Entities section. Click  Add.
- 4 In the Add dialog, in the Selections to add list, choose SCR Catalyst, ASC Catalyst, Mat Domain, Metal Shell Domain, Free Flow Domain, and Insulating Gas.
- 5 Click OK.

Now it is time to set up the physics interfaces that describe the mass transport, heat transfer, and fluid flow in the monolithic reactor. Optionally, in the Model Builder toolbar, click Collapse All  to get a better overview of the tree for the remainder of the model setup.

Transport of Diluted Species in Porous Media Interface

During the Generate Space-Dependent Model procedure several feature nodes were added along with the new physics interfaces. Now go through these features one by one and enter settings, and make sure that they are assigned to the proper domains and boundaries in the geometry.

- 1 In the Model Builder window, under Monolith Reactor Model click Transport of Diluted Species in Porous Media.
- 2 In the Settings window for Transport of Diluted Species in Porous Media, locate the Domain Selection section.
- 3 From the Selection list, choose Porous and Free Flow Domains.



The fluid will be modeled as compressible. This setting is available in the Laminar Flow interface. This means that the mass conservation equation should be of the conservative form. Choose this form from the Advanced Settings section in the mass transfer interface's settings window.

- 1 Click the Show More Options button in the Model Builder toolbar.
- 2 In the Show More Options dialog, in the tree, select the checkbox for the node Physics > Advanced Physics Options.
- 3 Click OK.
- 4 In the Settings window for Transport of Diluted Species in Porous Media, click to expand the Advanced Settings section.
- 5 From the Material balance form list, choose Conservative.

POROUS MEDIUM

In the Model Builder window, expand the Transport of Diluted Species in Porous Media node.

Fluid

The mass transport model for the monolith channels assumes that there is only diffusive mass transport in the axial direction of the reactor, here along the z -axis. This can be accomplished by specifying the diffusivity only in the first element of the diagonal diffusion matrix. This may be difficult to converge though, and a more robust alternative is to set the radial diffusivity to a very low value.

- 1 In the Model Builder window, expand the Porous Medium 1 node, then click Fluid 1.

2 In the Settings window for Fluid, locate the Diffusion section.

3 From the Source list, choose Material.

4 From the Fluid material list, choose Gas: Nitrogen Solvent.

For each species, change from Isotropic to Diagonal, for the Fluid diffusion coefficient.

5 From the list, choose Diagonal.

6 Specify the D_{F,cH_2O} matrix as

pp1mat1.df5.D11*0.0001	0
0	pp1mat1.df5.D11

7 From the list, choose Diagonal.

8 Specify the D_{F,cNH_3} matrix as

pp1mat1.df1.D11*0.0001	0
0	pp1mat1.df1.D11

9 From the list, choose Diagonal.

10 Specify the $D_{F,cNO}$ matrix as

pp1mat1.df2.D11*0.0001	0
0	pp1mat1.df2.D11

11 From the list, choose Diagonal.

12 Specify the D_{F,cNO_2} matrix as

pp1mat1.df3.D11*0.0001	0
0	pp1mat1.df3.D11

13 From the list, choose Diagonal.

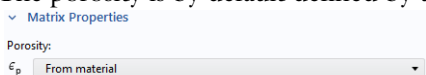
14 Specify the D_{F,cO_2} matrix as

pp1mat1.df4.D11*0.0001	0
0	pp1mat1.df4.D11

The entered expressions were set up by the Generate Material wizard and they can be found under the Global Definitions > Materials > Gas: Nitrogen node. D11 represents the zz-component in the diffusivity matrix.

Porous Matrix I

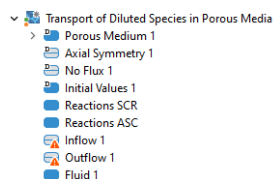
The porosity is by default defined by the Porous Material node.



INITIAL VALUES I

This model is highly nonlinear due to the reaction kinetics. In this case, starting from a nonreacting system leads to a more robust simulation. To achieve this set the initial concentration to zero.

In addition to the default feature nodes, the nodes Reactions 1, Inflow 1 and Outflow 1 were also added during the Generate Space-Dependent Model procedure. The Reaction feature gets input from the first Chemistry interface in the component. The inflow and outflow features' icons are marked with the warning sign  in the Model Builder window. The warning message, seen when placing the mouse pointer on top of the icons, reveals that they are empty and need to be assigned to the proper domains and boundaries in the geometry.



REACTIONS SCR

- 1 In the Model Builder window, under Monolith Reactor Model > Transport of Diluted Species in Porous Media click Reactions 1.
- 2 In the Settings window for Reactions, type Reactions SCR in the Label text field.
- 3 Locate the Domain Selection section. From the Selection list, choose SCR Catalyst.

REACTIONS ASC

- 1 In the Physics toolbar, click  Domains and choose Reactions.
- 2 In the Settings window for Reactions, type Reactions ASC in the Label text field.
- 3 Locate the Domain Selection section. From the Selection list, choose ASC Catalyst.
- 4 Locate the Reaction Rates section. From the Chemistry list, choose Chemistry: ASC (chem2).
- 5 Expand the Reacting Volume section and select Pore volume to specify the region where the reactions occur.

- 6 Drag the Reactions SCR node and place it below Reactions SCR.

INFLOW I

- 1 In the Model Builder window, click Inflow 1.
- 2 In the Settings window for Inflow, locate the Boundary Selection section.
- 3 From the Selection list, choose Flow Inlet.
- 4 Locate the Concentration section. In the c_{0,cH_2O} text field, type cH_2O_in .
- 5 In the c_{0,cNH_3} text field, type cNH_3_in .
- 6 In the $c_{0,cNO}$ text field, type cNO_in .
- 7 In the c_{0,cNO_2} text field, type cNO_2_in .
- 8 In the c_{0,cO_2} text field, type cO_2_in .

OUTFLOW I

- 1 In the Model Builder window, click Outflow 1.
- 2 In the Settings window for Outflow, locate the Boundary Selection section.
- 3 From the Selection list, choose Flow Outlet.

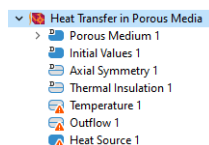
FLUID I

Next, add a Fluid feature to model the mass transfer in the free-flowing domain between the two catalysts. Use the diffusion coefficients defined by the nitrogen material.

- 1 In the Physics toolbar, click  Domains and choose Fluid.
- 2 In the Settings window for Fluid, locate the Domain Selection section.
- 3 From the Selection list, choose Free Flow Domain.
- 4 Locate the Diffusion section. From the Material list, choose Gas: Nitrogen Solvent.
- 5 From the D_{cH_2O} list, choose Diffusion coefficient, water in nitrogen (solvent) 5.
- 6 From the D_{cNH_3} list, choose Diffusion coefficient, ammonia in nitrogen (solvent) 1.
- 7 From the D_{cNO} list, choose Diffusion coefficient, nitrogen oxide in nitrogen (solvent) 2.
- 8 From the D_{cNO_2} list, choose Diffusion coefficient, no2 in nitrogen (solvent) 3.
- 9 From the D_{cO_2} list, choose Diffusion coefficient, oxygen in nitrogen (solvent) 4.

Heat Transfer in Porous Media

Next, set up the Heat Transfer in Porous Media interface. Similarly to the procedure used for the mass transfer interface, go through the generated feature nodes, modify and add as needed.



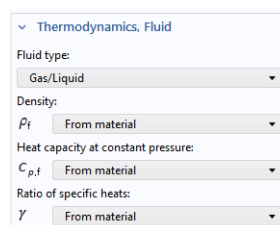
- 1 In the Model Builder window, under Monolith Reactor Model click Heat Transfer in Porous Media.
- 2 In the Settings window for Heat Transfer in Porous Media, locate the Domain Selection section.
- 3 From the Selection list, choose Heat Transfer Domains.

FLUID 1

Begin by specifying settings for convective and conductive heat transfer in the monolith channels.

- 1 In the Model Builder window, expand the Porous Medium 1 node, then click Fluid 1.
- 2 In the Settings window for Fluid, locate the Heat Conduction, Fluid section.
- 3 From the k_f list, choose From material.
- 4 Locate the Thermodynamics, Fluid section. From the ρ_f list, choose From material.
- 5 From the $C_{p,f}$ list, choose From material.
- 6 From the γ list, choose From material.

Note that the fluid properties are now defined by the Fluid subnode of the [Porous Material](#).



POROUS MATRIX 1

- 1 In the Model Builder window, click Porous Matrix 1.
- 2 In the Settings window for Porous Matrix, locate the Matrix Properties section.
- 3 From the Define list, choose Solid phase properties.
- 4 Locate the Heat Conduction, Porous Matrix section. From the k_s list, choose User defined. From the list, choose Diagonal.

Specifying the diagonal thermal conductivity elements allows you to represent anisotropic conductive heat transfer in the monolith channels.

5 Specify the k_s matrix as

ks_radial	0
0	ks_axial

Note that apart from the conductivity, the matrix properties are defined by the [Solid: Monolith Material](#) node added to the Porous Material feature.

INITIAL VALUES I

- 1 In the Model Builder window, under Monolith Reactor Model > Heat Transfer in Porous Media click Initial Values 1.
- 2 In the Settings window for Initial Values, locate the Initial Values section.
- 3 In the T text field, type $T_{\text{gas_in}}$. This parameter was previously defined in [Parameters: Temperature and Monolith Parameters](#).

TEMPERATURE I

- 1 In the Model Builder window, click Temperature 1.
- 2 Select Boundary 18 only.

OUTFLOW I

- 1 In the Model Builder window, click Outflow 1.
- 2 In the Settings window for Outflow, locate the Boundary Selection section.
- 3 From the Selection list, choose Flow Outlet.

HEAT SOURCE I

Couple the Heat Source to the heat source defined by the Transport of Diluted Species in Porous Media interface. The heat source defined in this interface already accounts for the porosity and various chemical reactions on the different catalyst domains. For this coupling, it is important that the domain selections match between the Heat Source node and the Transport of Dilute Species in Porous Media Interface.

- 1 In the Model Builder window, under Monolith Reactor Model> Heat Transfer in Porous Media click Heat Source 1.
- 2 Locate the Domain Selection section. From the Selection list, choose Porous and Free Flow Domains.
- 3 From the Material type list, choose From material.
- 4 Locate the Heat Source section. From the Q_0 list, choose Heat source (tds).

Continue by adding the features needed to describe the inflow boundary condition, the fluid domains, temperature boundary conditions, solid domains, porous domain, and the heat flux boundary conditions.

INFLOW 1

- 1 In the Physics toolbar, click  Boundaries and choose Inflow.
- 2 In the Settings window for Inflow, locate the Boundary Selection section.
- 3 From the Selection list, choose Flow Inlet.
- 4 Locate the Upstream Properties section. In the T_{ustr} text field, type `T_gas_in`.

FLUID 1

- 1 In the Physics toolbar, click  Domains and choose Fluid.
- 2 In the Settings window for Fluid, locate the Domain Selection section.
- 3 From the Selection list, choose Free Flow Domain.
- 4 Locate the Thermodynamics, Fluid section. From the Fluid type list, choose Gas/Liquid.

FLUID 2

- 1 In the Physics toolbar, click  Domains and choose Fluid.
- 2 Click in the Graphics window and then press Ctrl+A to select all domains.
- 3 In the Settings window for Fluid, locate the Domain Selection section.
- 4 From the Selection list, choose Insulating Gas.

Next, add a temperature boundary condition at the metal wall of the reactor upstream of the SCR catalyst. We assume that the temperature is the same as that of the inlet gas.

TEMPERATURE 2

- 1 In the Physics toolbar, click  Boundaries and choose Temperature.
- 2 Select Boundaries 17, 48, and 51 only.
- 3 In the Settings window for Temperature, locate the Temperature section.
- 4 In the T_0 text field, type `T_gas_in`.

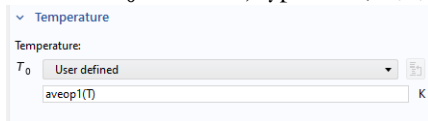
We also have to define the temperature for the reactor wall downstream of the ASC catalyst. We assume that the temperature is that of the gas exiting the ASC catalyst. Add a feature to derive the average temperature of the outlet gas, and assign it to the boundary.

AVERAGE I (AVEOP1)

- 1 In the Definitions toolbar, click  Nonlocal Couplings and choose Average.
- 2 In the Settings window for Average, locate the Source Selection section.
- 3 From the Geometric entity level list, choose Boundary.
- 4 Select Boundaries 6 and 45 only.

TEMPERATURE 3

- 1 In the Physics toolbar, click  Boundaries and choose Temperature.
- 2 Select Boundaries 14, 16, 45, and 50 only.
- 3 In the Settings window for Temperature, locate the Temperature section.
- 4 In the T_0 text field, type aveop1(T).



Add a Solid feature to describe the heat transfer in the metal shell.

SOLID I

- 1 In the Physics toolbar, click  Domains and choose Solid.
- 2 In the Settings window for Solid, locate the Domain Selection section.
- 3 From the Selection list, choose Metal Shell Domain.

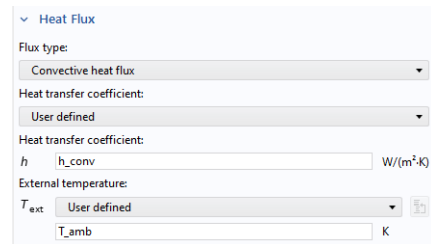
Add a Heat Flux feature to describe the heat transfer from the reactor exterior surface to the surrounding air.

HEAT FLUX I

- 1 In the Physics toolbar, click  Boundaries and choose Heat Flux.
- 2 Select Boundaries 31–34 and 70 only.
- 3 In the Settings window for Heat Flux, locate the Material Type section.
- 4 From the Material type list, choose From material.
- 5 Locate the Heat Flux section. From the Flux type list, choose Convective heat flux.
- 6 In the h text field, type h_conv.

7 In the T_{ext} text field, type T_{amb} .

Add another Heat Flux feature to describe the heat transfer from the reactor outlet surface to the surrounding air.



HEAT FLUX 2

- 1 In the Physics toolbar, click  Boundaries and choose Heat Flux.
- 2 Select Boundary 15 only.
- 3 In the Settings window for Heat Flux, locate the Material Type section.
- 4 From the Material type list, choose Solid.
- 5 Locate the Heat Flux section. From the Flux type list, choose Convective heat flux.
- 6 In the h text field, type $1[\text{W}/(\text{m}^2\cdot\text{K})]$.
- 7 In the T_{ext} text field, type T_{amb} .

The final feature that is needed to describe the heat transfer in the system is a Porous Medium feature for the supportive mat domain. The fluid in the mat is, for the simplicity of this example, assumed to be exhaust gas. This is a fair assumption, and this way we can take the fluid properties from the material.

POROUS MEDIUM 2

- 1 In the Physics toolbar, click  Domains and choose Porous Medium.
- 2 In the Model Builder window, click Porous Medium 2.
- 3 Select Domain 14 only.

Fluid 1

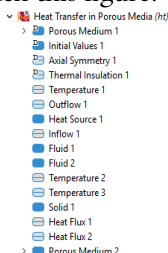
- 1 In the Model Builder window, click Fluid 1.
- 2 In the Settings window for Fluid, locate the Thermodynamics, Fluid section.
- 3 From the γ list, choose From material.

Porous Matrix 1

- 1 In the Model Builder window, click Porous Matrix 1.
- 2 In the Settings window for Porous Matrix, locate the Matrix Properties section.
- 3 From the ϵ_p list, choose User defined. In the associated text field, type 0.5.
- 4 Locate the Heat Conduction, Porous Matrix section. From the k_b list, choose User defined. In the associated text field, type 0.1.

- 5 Locate the Thermodynamics, Porous Matrix section. From the ρ_b list, choose User defined. In the associated text field, type $0.63[\text{g}/\text{cm}^3]$.
- 6 From the $C_{p,b}$ list, choose User defined. In the associated text field, type $1.1[\text{J}/\text{g}/\text{degC}]$.

The node sequence in the Model Builder under the Heat Transfer in Porous Media interface should now match this figure:



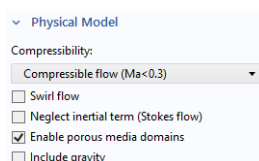
Having finished setting up the heat transfer physics, proceed to set up the Laminar Flow interface. Model the fluid as compressible, and assume that the flow is laminar both inside the channels and in the free-flow domain between the catalysts.

Laminar Flow

- 1 In the Model Builder window, under Monolith Reactor Model click Laminar Flow
- 2 In the Settings window for Laminar Flow, locate the Domain Selection section.
- 3 From the Selection list, choose Porous and Free Flow Domains.
- 4 Locate the Physical Model section. From the Compressibility list, choose Compressible flow ($\text{Ma} < 0.3$).
- 5 Select the Enable porous media domains checkbox.

FLUID PROPERTIES I

- 1 In the Model Builder window, expand the Laminar Flow node, then click Fluid Properties 1.
- 2 In the Settings window for Fluid Properties, locate the Fluid Properties section.
- 3 From the μ list, choose From material.



WALL 1

- 1 In the Model Builder window, click Wall 1.
- 2 In the Settings window for Wall, locate the Boundary Condition section.
- 3 From the Wall condition list, choose Slip.

INLET 1

- 1 In the Model Builder window, click Inlet 1.
- 2 In the Settings window for Inlet, locate the Boundary Selection section.
- 3 From the Selection list, choose Flow Inlet.
- 4 Locate the Boundary Condition section. From the list, choose Mass flow.
- 5 Locate the Mass Flow section. In the m text field, type `m_tot_in`.

OUTLET 1

- 1 In the Model Builder window, click Outlet 1.
- 2 In the Settings window for Outlet, locate the Boundary Selection section.
- 3 From the Selection list, choose Flow Outlet.

POROUS MEDIUM 1

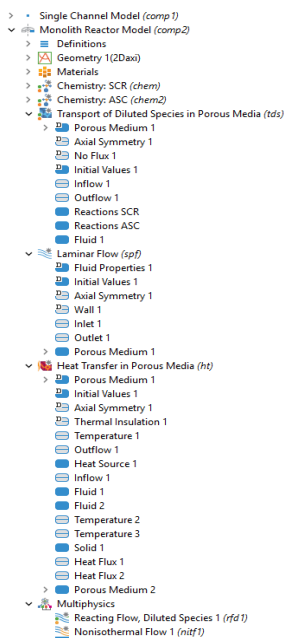
- 1 In the Physics toolbar, click  Domains and choose Porous Medium.
- 2 Select Domains 3 and 5 only.

POROUS MATRIX 1

- 1 In the Model Builder window, click Porous Matrix 1.
- 2 In the Settings window for Porous Matrix, locate the Matrix Properties section.
- 3 From the κ list, choose User defined. From the list, choose Diagonal.
- 4 Specify the κ matrix as

κ_{radial}	0
0	κ_{axial}

The sequence of nodes for the 2D axisymmetric Model in the Model Builder should match this figure.



Before solving the problem numerically, the geometry needs to be discretized with a mesh.

Mesh

Use a Free Triangular mesh for the supportive mat, the metal shell, and the insulating air, and use a mapped mesh for the monoliths. Finally, add a boundary layer mesh to the monoliths, the mat, and the free flow domain.

- 1 In the Model Builder window, under Monolith Reactor Model click Mesh 1.
- 2 In the Settings window for Mesh, locate the Sequence Type section.
- 3 From the list, choose User-controlled mesh.

SIZE

- 1 In the Model Builder window, under Monolith Reactor Model > Mesh 1 click Size.
- 2 In the Settings window for Size, locate the Element Size section.
- 3 From the Predefined list, choose Coarser.

SIZE 1

- 1 In the Mesh toolbar, click  Sizing and choose Size.
- 2 Drag and drop below Size.
- 3 In the Settings window for Size, locate the Geometric Entity Selection section.
- 4 From the Geometric entity level list, choose Domain.
- 5 Select Domain 4 only.
- 6 Locate the Element Size section. From the Calibrate for list, choose Fluid dynamics.
- 7 From the Predefined list, choose Finer.

MAPPED 1

- 1 In the Mesh toolbar, click  Mapped.
- 2 In the Settings window for Mapped, locate the Domain Selection section.
- 3 From the Geometric entity level list, choose Domain.
- 4 From the Selection list, choose ASC Catalyst.
- 5 Click  Clear Selection.
- 6 Select Domains 3 and 5 only.

DISTRIBUTION 1

- 1 In the Mesh toolbar, click  Distribution.
- 2 Select Boundaries 6, 8, 10, and 12 only.
- 3 In the Settings window for Distribution, locate the Distribution section.
- 4 From the Distribution type list, choose Predefined.
- 5 In the Number of elements text field, type 20.
- 6 In the Element ratio text field, type 3.

DISTRIBUTION 2

- 1 In the Mesh toolbar, click  Distribution.
- 2 Select Boundaries 9 and 47 only.
- 3 In the Settings window for Distribution, locate the Distribution section.
- 4 From the Distribution type list, choose Predefined.
- 5 In the Number of elements text field, type 80.
- 6 In the Element ratio text field, type 10.
- 7 Select the Symmetric distribution checkbox.

DISTRIBUTION 3

- 1 In the Mesh toolbar, click  Distribution.
- 2 Select Boundaries 5 and 44 only.
- 3 In the Settings window for Distribution, locate the Distribution section.
- 4 From the Distribution type list, choose Predefined.
- 5 In the Number of elements text field, type 20.
- 6 In the Element ratio text field, type 3.
- 7 Select the Symmetric distribution checkbox.

DISTRIBUTION 4

In the Mesh toolbar, click  Distribution.

SIZE 1

- 1 In the Model Builder window, right-click Free Triangular 1 and choose Size.
- 2 In the Settings window for Size, locate the Geometric Entity Selection section.
- 3 From the Geometric entity level list, choose Domain.
- 4 Select Domain 7 only.

BOUNDARY LAYERS 1

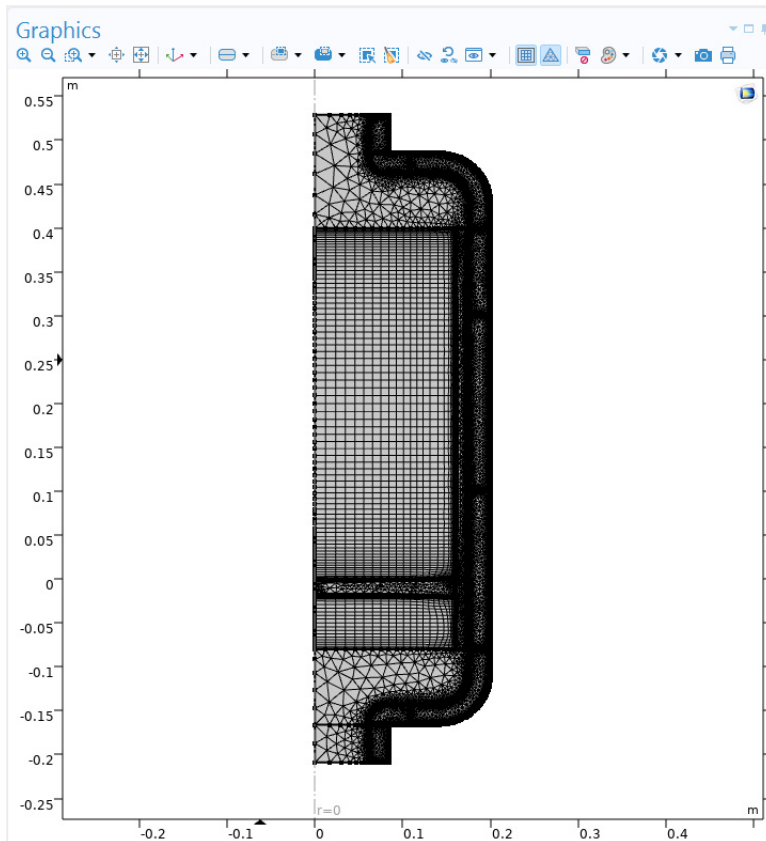
- 1 In the Mesh toolbar, click  Boundary Layers.
- 2 Drag and drop below Boundary Layers 1.
- 3 In the Settings window for Boundary Layers, locate the Domain Selection section.
- 4 From the Geometric entity level list, choose Domain.
- 5 Select Domains 3–5 and 14 only.

BOUNDARY LAYER PROPERTIES

- 1 In the Model Builder window, click Boundary Layer Properties.
- 2 Select Boundaries 8, 10, 44, 46, and 47 only.
- 3 In the Settings window for Boundary Layer Properties, locate the Layers section.
- 4 In the Number of layers text field, type 6.
- 5 In the Stretching factor text field, type 1.3.

BOUNDARY LAYERS I

- 1 In the Model Builder window, click Boundary Layers 1.
- 2 Drag and drop below Free Triangular 1.
- 3 In the Settings window for Boundary Layers, click  Build All, then click the Zoom Extents button  in the Graphics toolbar to view the entire geometry.



Study 5: Monolith Reactor Model

Set up the study to solve for each of the engine load cases using a Parametric Sweep study step. A separate study step is used to first solve for the fluid flow to provide good initial values for the full coupled problem.

- 1 In the Model Builder window, click Study 5.

- 2 In the Settings window for Study, type Study 5: Monolith Reactor Model in the Label text field.

STEP 1: STATIONARY

- 1 In the Model Builder window, expand the Study 5: Monolith Reactor Model node, then click Step 1: Stationary.
- 2 In the Settings window for Stationary, locate the Physics and Variables Selection section.
- 3 Set up this step to only solve for fluid flow. Use the Solve for column to clear the checkboxes for Chemistry: SCR, Chemistry: ASC, Transport of Diluted Species in Porous Media, and Heat Transfer in Porous Media.
- 4 Also clear the checkboxes for Reacting Flow, Diluted Species 1 and Nonisothermal Flow 1 under Monolith Reactor Model > Multiphysics.

Node	Solve for	Equation form
Single Channel Model	☐	
Selective Catalytic Reduction Catalyst...	☐	Automatic (Time dependent)
Ammonia Slip Catalyst (ASC)	☐	Automatic (Time dependent)
Monolith Reactor Model	☒	
Chemistry: SCR	☐	Automatic (Stationary)
Chemistry: ASC	☐	Automatic (Stationary)
Transport of Diluted Species in Porous...	☐	Automatic (Stationary)
Laminar Flow	☒	Automatic (Stationary)
Heat Transfer in Porous Media	☐	Automatic (Stationary)
Multiphysics		
Reacting Flow, Diluted Species 1	☐	Automatic (Stationary)
Nonisothermal Flow 1	☐	Automatic (Stationary)

STEP 2: STATIONARY 2

In the Study toolbar, click  Study Steps and choose Stationary > Stationary.

PARAMETRIC SWEEP

- 1 In the Study toolbar, 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)

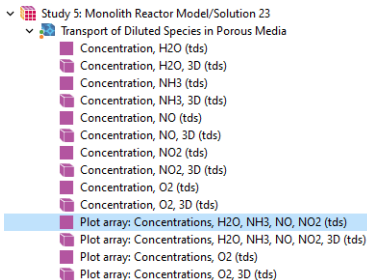
- 6 In the Model Builder window, click Study 5: Monolith Reactor Model.

- 7 In the Settings window for Study, locate the Study Settings section.
- 8 For this model the plots will be created from results templates. Clear the Generate default plots checkbox.
- 9 In the Study toolbar, click  Compute.

The following steps generate [Figure 13](#), [Figure 14](#), and [Figure 15](#). Using a Result Template is an efficient way to create plots. Add the template and then modify it if necessary.

Result Templates

- 1 In the Results toolbar, click  Result Templates to open the Result Templates window.
- 2 Go to the Result Templates window.
- 3 In the tree, select Plot array: Concentrations, H2O, NH3, NO, NO2 (tds) under Study 5: Monolith Reactor Model/Solution 23 > Transport of Diluted Species in Porous Media >



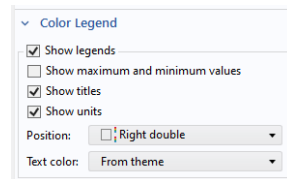
- 4 Click the Add Result Template button in the window toolbar.

Results for Study 5

FIGURE 13: NITROGEN SPECIES MOLAR FRACTIONS

- 1 In the Settings window for 2D Plot Group, type Nitrogen Species Molar Fractions in the Label text field.
- 2 Locate the Data section. From the Dataset list, choose Study 5: Monolith Reactor Model/Parametric Solutions 5 (sol25).
- 3 From the Cases list, choose Low Load.

- 4 Click to expand the Title section. From the Title type list, choose None.
- 5 Locate the Color Legend section. From the Position list, choose Right double.
- 6 In the Model Builder window, expand the node Nitrogen Species Molar Fractions.
- 7 In the Model Builder window, under Results > Nitrogen Species Molar Fractions, Ctrl-click to select Surface, H₂O, Total Flux, H₂O, H₂O, Total Flux, NH₃, Total Flux, NO, and Total Flux, NO₂.
- 8 Right-click and choose Delete.



Surface, NH₃ (SCR)

- 1 In the Settings window for Surface, type Surface, NH₃ (SCR) in the Label text field.
- 2 Locate the Expression section. In the Expression text field, type y_{NH_3} .
- 3 From the Unit list, choose ppm.
- 4 Locate the Coloring and Style section. From the Color table list, choose Cyanthus.
- 5 In the Color legend title text field, type NH_3 (SCR).
- 6 From the Color table type list, choose Discrete.
- 7 In the Number of bands text field, type 20.
- 8 Right-click Surface, NH₃ (SCR) and choose Selection.
- 9 Click the  Zoom Extents button in the Graphics toolbar.
- 10 Select Domain 5 only.
- 11 In the Model Builder window, click Surface, NH₃ (SCR).
- 12 In the Settings window for Surface, type Surface, NH₃ (SCR) in the Label text field.

Surface, NH₃ (ASC)

- 1 Right-click Surface, NH₃ (SCR) and choose Duplicate.
- 2 In the Settings window for Surface, type Surface, NH₃ (ASC) in the Label text field.
- 3 Locate the Coloring and Style section. In the Color legend title text field, type NH_3 (ASC).
- 4 In the Model Builder window, expand the Surface, NH₃ (ASC) node, then click Selection 1.
- 5 In the Settings window for Selection, locate the Selection section.

- 6 Click to select the  Activate Selection toggle button.
- 7 Select Domain 3 only.

Surface, NO (SCR)

- 1 In the Model Builder window, under Results > Nitrogen Species Molar Fractions click Surface, NO.
- 2 In the Settings window for Surface, locate the Expression section.
- 3 In the Expression text field, type y_{NO} .
- 4 From the Unit list, choose ppm.
- 5 Locate the Coloring and Style section. From the Color table list, choose Baptisia.
- 6 In the Color legend title text field, type NO (SCR).
- 7 From the Color table type list, choose Discrete.
- 8 In the Number of bands text field, type 20.
- 9 In the Model Builder window, click Surface, NO.
- 10 In the Label text field, type Surface, NO (SCR).
- 11 Right-click Surface, NO (SCR) and choose Selection.
- 12 Select Domain 5 only.

Surface, NO (ASC)

- 1 In the Model Builder window, right-click Surface, NO (SCR) and choose Duplicate.
- 2 In the Settings window for Surface, type Surface, NO (ASC) in the Label text field.
- 3 Locate the Coloring and Style section. In the Color legend title text field, type NO (ASC).
- 4 In the Model Builder window, expand the Surface, NO (ASC) node, then click Selection 1.
- 5 In the Settings window for Selection, locate the Selection section.
- 6 Click to select the  Activate Selection toggle button.
- 7 Select Domain 3 only.

Surface, NO2 (SCR)

- 1 In the Model Builder window, under Results > Nitrogen Species Molar Fractions click Surface, NO2.
- 2 In the Settings window for Surface, type Surface, NO2 (SCR) in the Label text field.

- 3 Locate the Expression section. In the Expression text field, type y_{NO_2} .
- 4 From the Unit list, choose ppm.
- 5 Locate the Coloring and Style section. From the Color table list, choose Arctium.
- 6 In the Color legend title text field, type NO_2 (SCR).
- 7 From the Color table type list, choose Discrete.
- 8 In the Number of bands text field, type 20.
- 9 Right-click Surface, NO_2 (SCR) and choose Selection.
- 10 Select Domain 5 only.

Surface, NO_2 (ASC)

- 1 Right-click Surface, NO_2 (SCR) and choose Duplicate.
- 2 In the Settings window for Surface, type Surface, NO_2 (ASC) in the Label text field.
- 3 Locate the Coloring and Style section. In the Color legend title text field, type NO_2 (ASC).
- 4 In the Model Builder window, under Results > Nitrogen Species Molar Fractions > Surface, NO_2 (ASC) click Selection 1.
- 5 In the Settings window for Selection, locate the Selection section.
- 6 Click to select the  Activate Selection toggle button.
- 7 Select Domain 3 only.
- 8 Click the  Zoom Extents button in the Graphics toolbar.
- 9 In the Nitrogen Species Molar Fractions toolbar, click  Plot.

NH₃

- 1 In the Model Builder window, click NH₃.
- 2 In the Settings window for Annotation, locate the Annotation section.
- 3 In the Text field, type NH₃\$_3\$.
- 4 Select the LaTeX markup checkbox.
- 5 Click to expand the Plot Array section. In the Index text field, type 0.

NO

- 1 In the Model Builder window, click NO.
- 2 In the Settings window for Annotation, locate the Annotation section.
- 3 Click to expand the Plot Array section. In the Index text field, type 1.

NO₂

- 1 In the Model Builder window, click NH₃.
- 2 In the Settings window for Annotation, locate the Annotation section.
- 3 In the Text field, type NO₂\$.
- 4 Select the LaTeX markup checkbox.
- 5 Click to expand the Plot Array section. In the Index text field, type 2.

Nitrogen Species Molar Fractions

Switch between the three cases to see the different results.

- 1 In the Model Builder window, under Results click Nitrogen Species Molar Fractions.
- 2 In the Settings window for 2D Plot Group, locate the Data section.
- 3 From the Cases list, choose Intermediate Load.
- 4 In the Nitrogen Species Molar Fractions toolbar, click  Plot.
- 5 From the Cases list, choose High Load.
- 6 In the Nitrogen Species Molar Fractions toolbar, click  Plot.

The following steps generate [Figure 16](#).

FIGURE 16: T, U, AND dP

- 1 In the Results toolbar, click  2D Plot Group.
- 2 In the Settings window for 2D Plot Group, type Drive Cases, ANR = 1.3, T, U, and dP in the Label text field.
- 3 Locate the Data section. From the Dataset list, choose Study 5: Monolith Reactor Model/Parametric Solutions 5 (sol25).
- 4 Locate the Title section. From the Title type list, choose None.
- 5 Locate the Color Legend section. Select the Show titles checkbox.
- 6 Select the Show units checkbox.
- 7 Click to expand the Plot Array section. Select the Enable checkbox.

Velocity

- 1 In the Drive Cases, ANR = 1.3, T, U, and dP toolbar, click  Surface.
- 2 In the Settings window for Surface, type Velocity in the Label text field.
- 3 Locate the Expression section. In the Expression text field, type $\text{spf} \cdot U$.
- 4 Locate the Coloring and Style section. From the Color table list, choose Metasepia.
- 5 In the Color legend title text field, type U.

- 6 From the Color table transformation list, choose Reverse.
- 7 From the Color table type list, choose Discrete.
- 8 In the Number of bands text field, type 5.
- 9 In the Drive Cases, ANR = 1.3, T, U, and dP toolbar, click  Annotation.
- 10 In the Settings window for Annotation, type U in the Label text field.
- 11 Locate the Annotation section. In the Text text field, type U.
- 12 Locate the Position section. In the z text field, type -0.21.
- 13 Locate the Coloring and Style section. Clear the Show point checkbox.
- 14 Click to expand the Plot Array section. Select the Manual indexing checkbox.

Pressure

- 1 In the Drive Cases, ANR = 1.3, T, U, and dP toolbar, click  Surface.
- 2 In the Settings window for Surface, type Pressure in the Label text field.
- 3 Locate the Expression section. In the Expression text field, type p.
- 4 Locate the Coloring and Style section. From the Color table list, choose Agama.
- 5 In the Color legend title text field, type dP.
- 6 From the Color table type list, choose Discrete.
- 7 In the Drive Cases, ANR = 1.3, T, U, and dP toolbar, click  Annotation.
- 8 In the Settings window for Annotation, type dP in the Label text field.
- 9 Locate the Annotation section. In the Text text field, type dP.
- 10 Locate the Position section. In the z text field, type -0.21.
- 11 Locate the Coloring and Style section. Clear the Show point checkbox.
- 12 Locate the Plot Array section. Select the Manual indexing checkbox.
- 13 In the Index text field, type 1.

Temperature

- 1 In the Drive Cases, ANR = 1.3, T, U, and dP toolbar, click  Surface.
- 2 In the Settings window for Surface, type Temperature in the Label text field.
- 3 Locate the Expression section. In the Expression text field, type T.
- 4 From the Unit list, choose °C.
- 5 Locate the Coloring and Style section. From the Color table list, choose Plasma.
- 6 In the Color legend title text field, type T.
- 7 From the Color table type list, choose Discrete.

- 8 In the Drive Cases, ANR = 1.3, T, U, and dP toolbar, click  Selection.
- 9 In the Settings window for Selection, locate the Selection section.
- 10 From the Selection list, choose Porous and Free Flow Domains.
- 11 In the Drive Cases, ANR = 1.3, T, U, and dP toolbar, click  Annotation.
- 12 In the Settings window for Annotation, type T in the Label text field.
- 13 Locate the Annotation section. In the Text text field, type T.
- 14 Locate the Position section. In the z text field, type -0.21.
- 15 Locate the Coloring and Style section. Clear the Show point checkbox.
- 16 Locate the Plot Array section. Select the Manual indexing checkbox.
- 17 In the Index text field, type 2.
- 18 Click the  Zoom Extents button in the Graphics toolbar.
- 19 In the Drive Cases, ANR = 1.3, T, U, and dP toolbar, click  Plot.

The following steps generate [Figure 17](#).

FIGURE 17: CONVERSIONS, NH₃ AND NO_x

- 1 In the Results toolbar, click  1D Plot Group.
- 2 In the Settings window for 1D Plot Group, type Conversions, NH₃ and NO_x, All Cases in the Label text field.
- 3 Locate the Data section. From the Dataset list, choose Study 5: Monolith Reactor Model/Parametric Solutions 5 (sol25).
- 4 Click to expand the Title section. From the Title type list, choose None.
- 5 Locate the Plot Settings section.
- 6 Select the y-axis label checkbox. In the associated text field, type Conversion.

NH₃ center

- 1 In the Conversions, NH₃ and NO_x, All Cases toolbar, click  Line Graph.
- 2 In the Settings window for Line Graph, type NH₃ center in the Label text field.
- 3 Select Boundaries 5, 7, and 9 only.
- 4 Locate the y-Axis Data section. In the Expression text field, type x_{NH_3} .
- 5 Select the Description checkbox. In the associated text field, type Conversion.
- 6 Locate the x-Axis Data section. From the Parameter list, choose Expression.
- 7 In the Expression text field, type $(0.4-z)*\pi*d_{cat}^2/4$.
- 8 Select the Description checkbox. In the associated text field, type Volume.
- 9 Click to expand the Coloring and Style section. Find the Line style subsection. From the Line list, choose Cycle.

- 10 From the Color list, choose Blue.
- 11 From the Width list, choose 2.
- 12 Click to expand the Legends section. Select the Show legends checkbox.
- 13 Find the Prefix and suffix subsection. In the Prefix text field, type $\text{NH}_{3\text{ center}}$.

NO_x center

- 1 Right-click NH_3 center, and choose Duplicate.
- 2 In the Settings window for Line Graph, type NO_x center in the Label text field.
- 3 Select Boundaries 5, 7, and 9 only.
- 4 Locate the y-Axis Data section. In the Expression text field, type x_{NO_x} .
- 5 Locate the Coloring and Style section. Find the Line style subsection. From the Line list, choose Cycle (reset).
- 6 From the Color list, choose Magenta.
- 7 Locate the Legends section. Find the Prefix and suffix subsection. In the Prefix text field, type NO_x center.
- 8 In the Model Builder window, under Results > Conversions, NH_3 and NO_x , All Cases, Ctrl-click to select NH_3 center, and NO_x center.
- 9 Right-click and choose Duplicate.

NH₃ edge

- 1 In the Model Builder window, under Results > Conversions, NH_3 and NO_x , All Cases click NH_3 center, 1.
- 2 In the Settings window for Line Graph, type NH_3 edge in the Label text field.
- 3 Locate the Selection section. Click  Clear Selection.
- 4 Select Boundaries 44, 46, and 47 only.
- 5 Click to expand the Coloring and Style section. Find the Line style subsection. From the Line list, choose Cycle (reset).
- 6 From the Color list, choose Black.
- 7 Locate the Legends section. Find the Prefix and suffix subsection. In the Prefix text field, type $\text{NH}_{3\text{ edge}}$.

NO_x edge

- 1 In the Model Builder window, under Results > Conversions, NH_3 and NO_x , All Cases click NO_x center 1.
- 2 In the Settings window for Line Graph, type NO_x edge in the Label text field.
- 3 Locate the Selection section. Click  Clear Selection.

- 4 Select Boundaries 44, 46, and 47 only.
- 5 Locate the Coloring and Style section. From the Color list, choose Red.
- 6 Locate the Legends section. Find the Prefix and suffix subsection. In the Prefix text field, type NO_x edge, .
- 7 In the Model Builder window, click Conversions, NH_3 and NO_x , All Cases.
- 8 In the Settings window for 1D Plot Group, click to expand the Window Settings section.
- 9 Locate the Legend section. From the Layout list, choose Outside graph axis area.
- 10 Click the  Zoom Extents button in the Graphics toolbar.
- 11 In the Conversions, NH_3 and NO_x , All Cases toolbar, click  Plot.

The following steps generate [Figure 18](#).

FIGURE 18: TEMPERATURE DIFFERENCE ALONG REACTOR AXIS

- 1 In the Results toolbar, click  1D Plot Group.
- 2 In the Settings window for 1D Plot Group, type Temperature Difference Along Reactor Axis in the Label text field.
- 3 Locate the Data section. From the Dataset list, choose Study 5: Monolith Reactor Model/Parametric Solutions 5 (sol25).
- 4 Locate the Title section. From the Title type list, choose None.
- 5 Locate the Plot Settings section.
- 6 Select the x-axis label checkbox. In the associated text field, type Bed position along reactor axis (m).
- 7 Locate the Legend section. From the Layout list, choose Outside graph axis area.

Temperature At Reactor Center

- 1 Right-click Temperature Difference Along Reactor Axis and choose Line Graph.
- 2 In the Settings window for Line Graph, type Temperature At Reactor Center in the Label text field.
- 3 Select Boundaries 5, 7, and 9 only.
- 4 Locate the y-Axis Data section. In the Expression text field, type $T - T_{\text{gas_in}}$.
- 5 Locate the x-Axis Data section. From the Parameter list, choose Reversed arc length.
- 6 Locate the Coloring and Style section. From the Width list, choose 2.

- 7 Locate the Legends section. Select the Show legends checkbox.
- 8 Find the Prefix and suffix subsection. In the Prefix text field, type T_{center} , .

Temperature At Bed Edge

- 1 Right-click Temperature At Reactor Center and choose Duplicate.
- 2 In the Settings window for Line Graph, type Temperature At Bed Edge in the Label text field.
- 3 In the Settings window for Line Graph, locate the Selection section.
- 4 Click  Clear Selection.
- 5 Select Boundaries 44, 46, and 47 only.
- 6 Locate the Coloring and Style section. Find the Line style subsection. From the Line list, choose Dashed.
- 7 From the Color list, choose Cycle (reset).
- 8 From the Width list, choose 2.
- 9 Locate the Legends section. Find the Prefix and suffix subsection. In the Prefix text field, type T_{edge} , .
- 10 Click the  Zoom Extents button in the Graphics toolbar.
- 11 In the Temperature Difference Along Reactor Axis toolbar, click  Plot.

As a final evaluation, derive the average molar fraction of NH_3 and NO_x out from the first bed, as well as out from the reactor.

LINE AVERAGE SCR OUTLET

- 1 In the Results toolbar, click  More Derived Values and choose Average > Line Average.
- 2 In the Settings window for Line Average, type Line Average SCR Outlet in the Label text field.
- 3 Locate the Data section. From the Dataset list, choose Study 5: Monolith Reactor Model/Parametric Solutions 5 (sol25).
- 4 Select Boundary 10 only.
- 5 Locate the Expressions section. In the table, enter the following settings:

EXPRESSION	UNIT	DESCRIPTION
yNH3	ppm	Molar Fraction NH3
yNOx	ppm	Molar Fraction NOx

- 6 Click  next to  Evaluate, then choose New Table.

LINE AVERAGE REACTOR OUTLET

- 1 Right-click Line Average SCR Outlet and choose Duplicate.
- 2 In the Settings window for Line Average, type Line Average Reactor Outlet in the Label text field.
- 3 Select Boundary 6 only.
- 4 Click ▼ next to = Evaluate, then choose New Table.

The modeling instructions for the Concentration and Temperature Profiles plot is available in the Application Libraries' model `monolith_reactor.mph`.

