



Chemical Reaction Engineering

Simulations



Benelux

COMSOL BV
Röntgenlaan 37
2719 DX Zoetermeer
The Netherlands
☎ +31 (0) 79 363 4230
☎ +31 (0) 79 361 4212
✉ info@comsol.nl
🌐 www.comsol.nl

Denmark

COMSOL A/S
Diplomvej 381
2800 Kgs. Lyngby
☎ +45 88 70 82 00
☎ +45 88 70 80 90
✉ info@comsol.dk
🌐 www.comsol.dk

Finland

COMSOL OY
Arabiankatu 12
FIN-00560 Helsinki
☎ +358 9 2510 400
☎ +358 9 2510 4010
✉ info@comsol.fi
🌐 www.comsol.fi

France

COMSOL France
WTC, 5 pl. Robert Schuman
F-38000 Grenoble
☎ +33 (0)4 76 46 49 01
☎ +33 (0)4 76 46 07 42
✉ info@comsol.fr
🌐 www.comsol.fr

Germany

COMSOL Multiphysics GmbH
Berliner Str. 4
D-37073 Göttingen
☎ +49-551-99721-0
☎ +49-551-99721-29
✉ info@comsol.de
🌐 www.comsol.de

India

COMSOL Multiphysics Pvt. Ltd.
Esquire Centre,
C-Block, 3rd Floor
No. 9, M. G. Road
Bangalore 560001
Karnataka
☎ +91-80-4092-3859
☎ +91-80-4092-3856
✉ info@comsol.co.in

Italy

COMSOL S.r.l.
Via Vittorio Emanuele II, 22
25122 Brescia
☎ +39-030-3793800
☎ +39-030-3793899
✉ info.it@comsol.com
🌐 www.it.comsol.com

Norway

COMSOL AS
Postboks 5673 Sluppen
Søndre gate 7
NO-7485 Trondheim
☎ +47 73 84 24 00
☎ +47 73 84 24 01
✉ info@comsol.no
🌐 www.comsol.no

Sweden

COMSOL AB
Tegnérsgatan 23
SE-111 40 Stockholm
☎ +46 8 412 95 00
☎ +46 8 412 95 10
✉ info@comsol.se
🌐 www.comsol.se

Switzerland

COMSOL Multiphysics GmbH
Technoparkstrasse 1
CH-8005 Zürich
☎ +41 (0)44 445 2140
☎ +41 (0)44 445 2141
✉ info@ch.comsol.com
🌐 www.ch.comsol.com

United Kingdom

COMSOL Ltd.
UH Innovation Centre
College Lane
Hatfield
Hertfordshire AL10 9AB
☎ +44-(0)-1707 636020
☎ +44-(0)-1707 284746
✉ info.uk@comsol.com
🌐 www.uk.comsol.com

United States

COMSOL, Inc.
1 New England Executive Park
Suite 350
Burlington, MA 01803
☎ +1-781-273-3322
☎ +1-781-273-6603

COMSOL, Inc.
10850 Wilshire Boulevard
Suite 800
Los Angeles, CA 90024
☎ +1-310-441-4800
☎ +1-310-441-0868

COMSOL, Inc.
744 Cowper Street
Palo Alto, CA 94301
☎ +1-650-324-9935
☎ +1-650-324-9936
✉ info@comsol.com
🌐 www.comsol.com

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Chemical Reaction Engineering Simulations

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Version:

April 2011

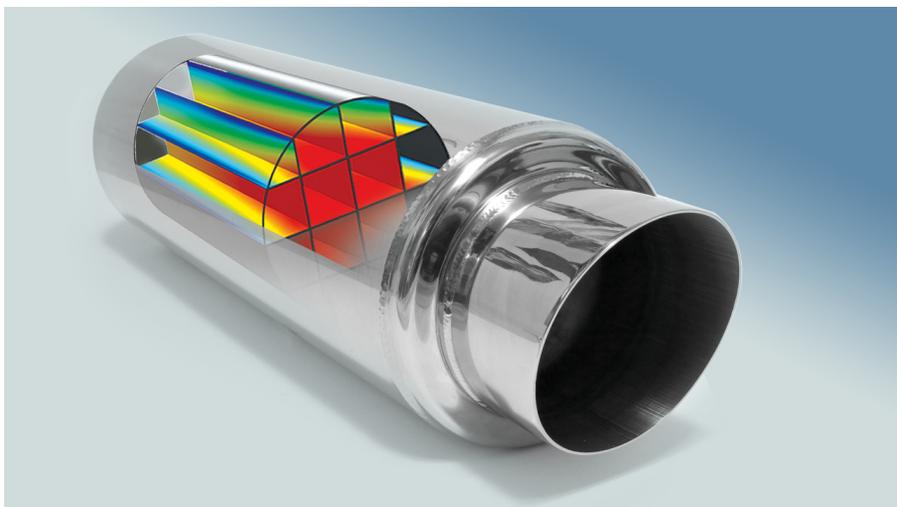
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Chemical Reaction Engineering Simulations

Simulations in chemical reaction engineering are used for different reasons 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.

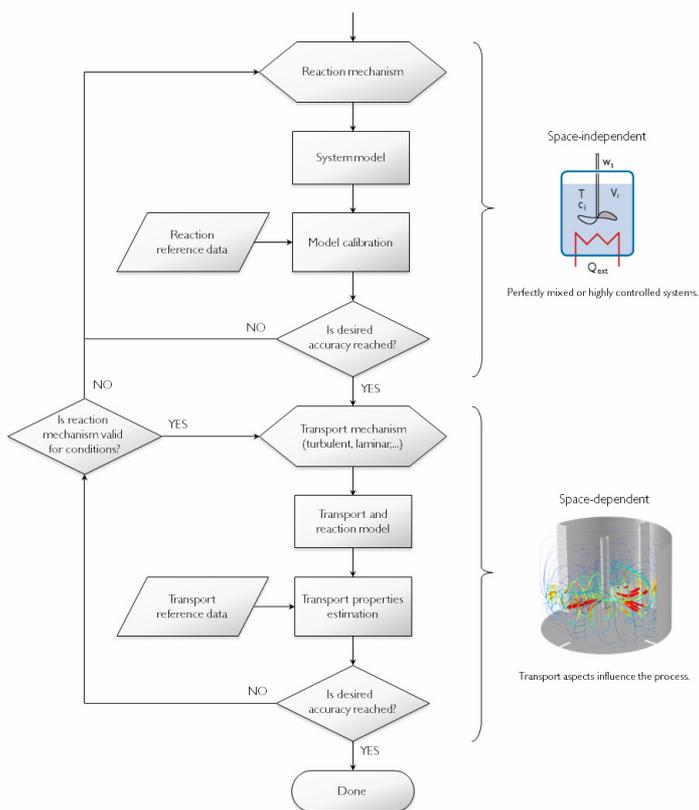
Once a process is well understood, modeling and simulations are used to optimize and control the process' variables and parameters. These 'virtual' experiments are run to adapt the process to different operating conditions.



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

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

This paper describes a strategy for modeling and simulating chemical reaction processes and systems and shown in this flowchart.



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

The strategy involves, firstly, 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 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 very 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 breadth, and are also subject to a range of external parameters including inflows, outflows, cooling, heating, and possible material loss. These are space (and time) dependent systems.

Investigating Chemical Reaction Kinetics—Modeling in Perfectly-mixed or Plug-flow Reactors

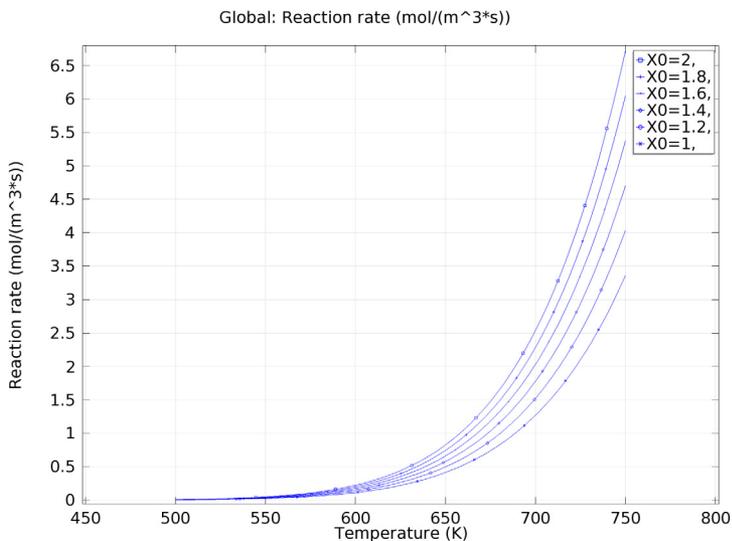
An important component in chemical reaction engineering is the definition of the respective reaction rate laws, which result from informed assumptions or hypotheses about the chemical reaction mechanisms. Ideally, a reaction mechanism and its corresponding rate laws are found through conducting rigidly-controlled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



Perfectly-mixed or ideal plug-flow reactors 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. Comparing these results to those from further experimental studies allows for 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.



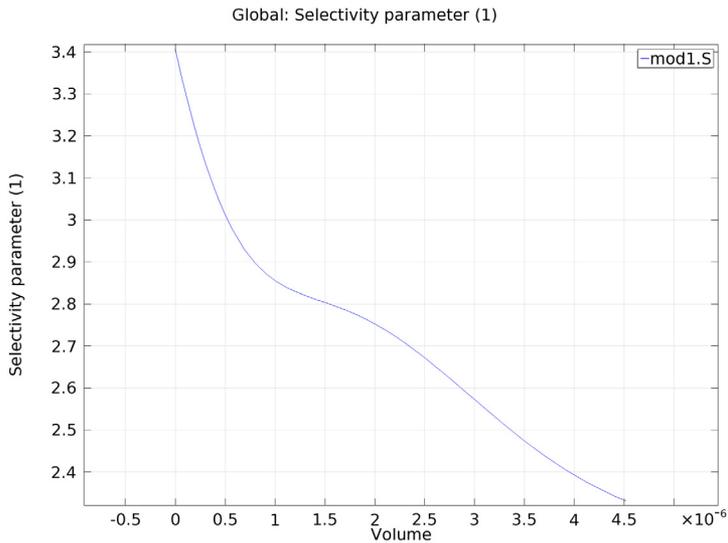
Reaction rate as a function of temperature as simulated in a perfectly-mixed reactor. The different lines represent different compositions of the reacting mixture.

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 then 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.



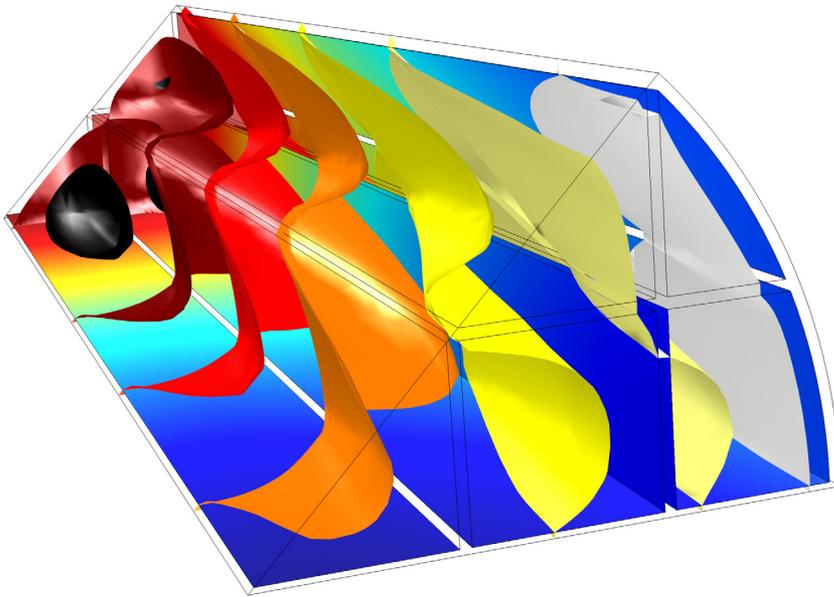
Depending on assumptions that can (or sometimes must) be made, these descriptions are done in either 1D, 2D, or 3D, where time-dependency can also be considered if it is of importance.



Reaction selectivity along the volume of a simulated 1D plug-flow reactor.

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

When its 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, along with the concrete results they provide, go towards developing or optimizing a chemical reactor with greater precision, or controlling a system with more confidence.



The temperature isosurfaces throughout a monolith reactor used in a catalytic converter. The surface plot shows the concentration profile of one of the reactants.

Example: Selective Reduction of Nitrogen Oxide in a Monolithic Reactor

Below is an example of a catalytic converter that removes nitrogen oxide from a car exhaust through the addition of ammonia. The example shows application of the above described modeling strategy, and demonstrates through a series of simulations how an understanding of this reactor and its system can be increased. To do this, it uses a number of the features found in the Chemical Reaction Engineering Module.

The Chemical Reaction Engineering Module

The Chemical Reaction Engineering Module (the Module) is tailor-made for the modeling of chemical systems primarily affected by chemical composition, reaction kinetics, fluid flow, and temperature. These properties can depend upon or be functions of space, time and the variables that describe them. The Module consists of a number of interfaces for the modeling of chemical reaction kinetics, mass transport in dilute, concentrated and electric potential-affected solutions, laminar and porous media flows, and energy transport.

It also provides access to a variety of ready-made expressions in order to calculate a system's thermodynamic and transport properties.

Introduction to the Example

This example illustrates the modeling of selective reduction of nitrogen oxide (NO) by a monolithic reactor in the exhaust system of an automobile. Exhaust gases from the engine pass through the channels of a monolithic reactor filled with a porous catalyst and, by adding ammonia (NH_3) to this stream, the NO can be selectively removed through a reduction reaction.

Yet, NH_3 is also oxidized in a parallel reaction, and the rates of the two reactions are affected by temperature as well as composition. This means that the amount of added NH_3 must exceed the expected amount of NO, while not being so excessive as to release NH_3 to the atmosphere.

The simulations are aimed at finding the optimal dosing of NH_3 , and investigating some of the other operating parameters in order to gauge their effects.



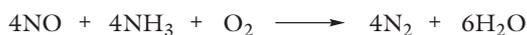
Catalytic converters reduce the NO_x levels in the exhaust gases emitted by combustion engines.

The example illustrates the modeling strategy described in the flowchart on page 4. First, the selectivity aspects of the kinetics are studied by modeling initial reaction rates as function of temperature and relative reactant amounts. Information from these studies will point to the general conditions required to attain the desired selectivity.

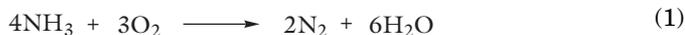
The reactor is then simplified and modeled as a non-isothermal plug flow reactor. This reveals the necessary NH_3 dosing levels based on the working conditions of the catalytic converter and assumed flowrate of NO in the exhaust stream. A 3D model of the catalytic converter is then set up and solved. This includes mass transport, heat transfer and fluid flow and provides insight and information for optimizing the dosing levels and other operational parameters.

Chemistry

Two parallel reactions occur in the $\text{V}_2\text{O}_5/\text{TiO}_2$ catalytic washcoat of the monolith reactor. The desired reaction is the reduction of NO by NH_3 :



However, NH_3 can, in parallel, undergo its own oxidation reaction:



The heterogeneous catalytic conversion of NO to N₂ is described by an Eley-Rideal mechanism. A key reaction step involves the reaction of NO in the gas phase with NH₃ that is adsorbed on the surface of the catalyst. Ref. 1 suggests the following reaction rate (mol/(m³·s)):

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

where

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

and

$$\alpha = A_0 \exp\left(-\frac{E_0}{R_g T}\right)$$

For Equation 1, the reaction rate (mol/(m³·s)) is given by

$$r_2 = k_2 c_{\text{NH}_3}$$

where

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

Investigating the Chemical Reaction Kinetics

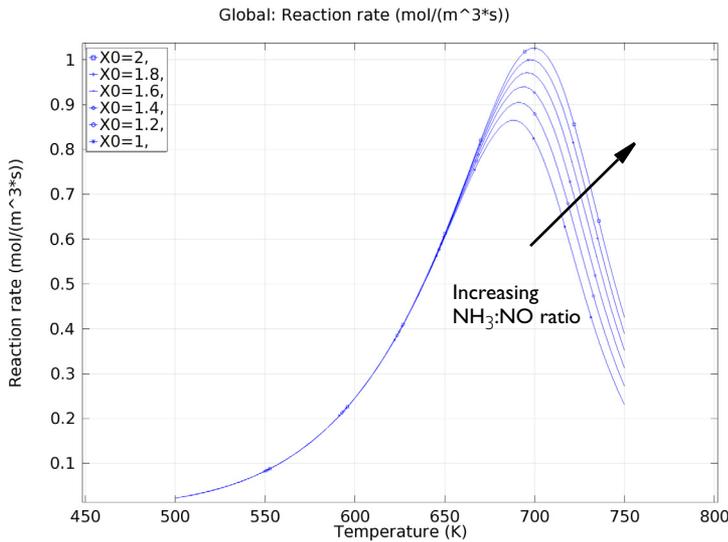
The competing chemical reactions raises the issue of optimally dosing NH₃ where stoichiometry suggests a 1:1 ratio of NH₃ to NO as the lower limit. Yet, excessively high levels of NH₃ leaving the catalytic converter should be avoided for reasons of both material costs and the environment.

Analyzing the kinetics helps to identify the conditions favoring the desirable reduction reaction while reducing the amount of NH₃ required to achieve this. Assuming the conditions of a perfectly-mixed reactor, the reaction rates of the reduction and oxidation reactions as a function of temperature and the relative amounts of each of the reactants are investigated.

The concentration of NO in the exhaust gas entering the catalytic converter is known to be 41.1 mmol/m³ while operating at an average speed of an automobile. The figure below shows the reaction rate of the NO reduction reaction as it is

affected by the temperature and the amount of NH_3 that has been added to the exhaust stream. What can be seen from the figure is that the reaction rate peaks at a temperature of around 700 K, depending on the amount of NH_3 that has been added, and that the reaction rate is benefited by a higher $\text{NH}_3:\text{NO}$ ratio.

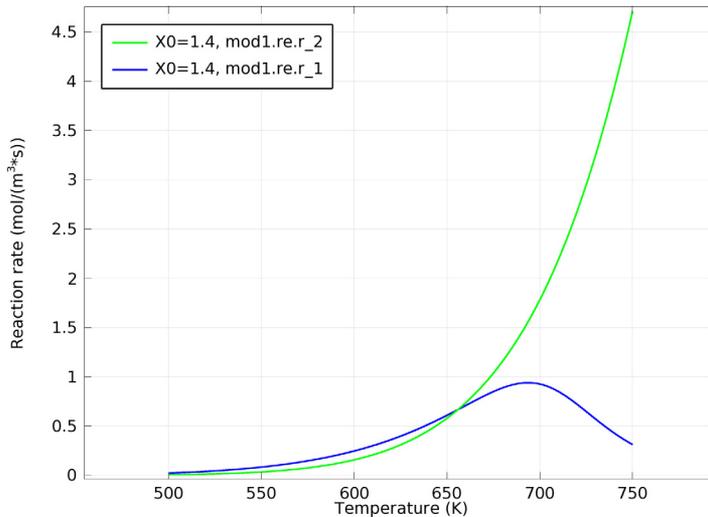
Higher concentrations of NH_3 in the gas phase leads to increased levels of surface-adsorbed NH_3 , favoring the conversion of NO to N_2 . Yet, at higher temperatures the NO reduction rate is decreased, which is explained by a faster desorption of NH_3 from the catalyst surface, and its subsequent oxidation.



Initial reaction rates of the NO reduction reaction (r_1) as a function of temperature. The $\text{NH}_3:\text{NO}$ ratio ranges from 1 to 2.

This figure gives no indication of the amount of NH_3 that is being released to the atmosphere, or the effects the NH_3 oxidation reaction has on the system, such as increasing the temperature and lowering the rate of NO reduction. The next figure simulates both reaction rates as a function of temperature, and indicates that

operating the monolith reactor at 700 K is not at all optimal. In fact, the NH_3 oxidation reaction takes over at about 660 K.



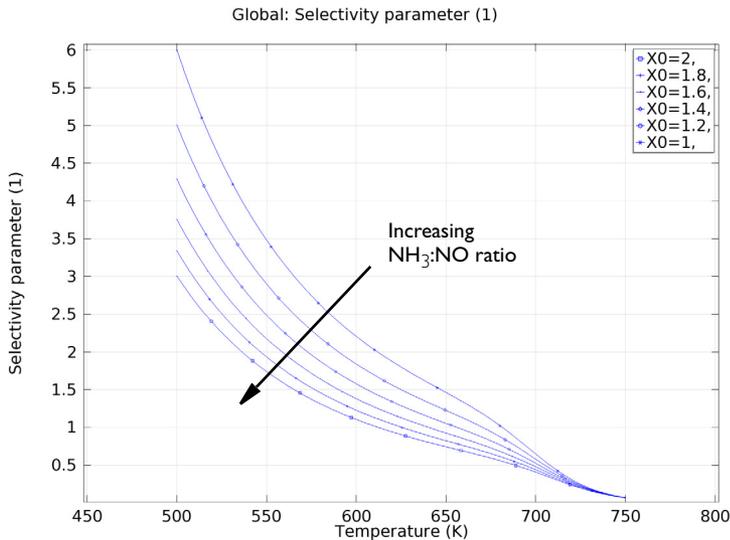
Reaction rates of the two competing reactions over increasing temperature: NO reduction (blue line) and NH_3 : oxidation (green line).

Selectivity is also a property that should be investigated at this stage and is given by the ratio

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

A value greater than 1 means that the NO reduction is favored and, according to the figure below, this is done in increasing measures at moderate temperatures and relatively low ratios of NH_3 :NO. This information together with that provided by the

previous figure, indicates that a more preferable operating temperature is somewhere between 500 K and 550 K.



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

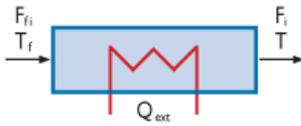
As the kinetic parameters were taken from the literature, these results should ideally be compared to an experiment simulating the same conditions. From here, these parameters could be fine-tuned.

Investigating a Plug-flow Reactor

None of the above, spatially-independent analyses provide information about the optimal dosing rate of NH_3 . To do this, a study must include spatial effects, particularly with respect to changing reactant concentrations and system temperature.

The catalytic converter consists of a series of long, but not particularly wide, channels bounded by walls impervious to mass transfer, although not heat transfer. Assuming

a constant velocity profile in the channel means that the system can be represented by a nonisothermal, plug flow reactor:



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

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

where F_i is the species molar flow rate (mol/s), V represents the reactor volume (m^3), and is R_i the species net reaction rate ($mol/(m^3 \cdot s)$). The energy balance for the ideal reacting gas is:

$$\sum_i F_i C_{p,i} \frac{dT}{dV} = Q_{ext} + Q \quad (2)$$

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

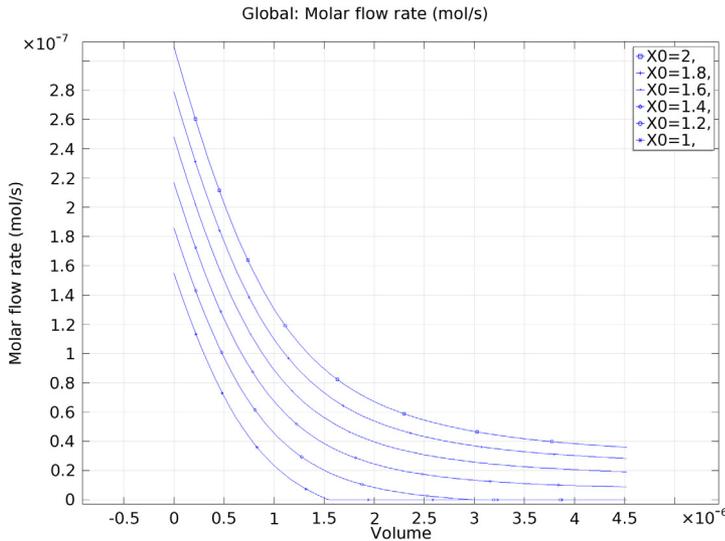
$$Q = -\sum_j H_j r_j$$

where H_j the heat of reaction (J/mol), and r_j the reaction rate ($mol/(m^3 \cdot s)$).

The reactor equations are solved for a channel 0.36 m in length with a cross sectional area of 12.6 mm^2 . The operating conditions for this example are such that the exhaust gas contains 41.1 mmol/m^3 of NO at a temperature of 523 K passing through the channel at 0.3 m/s.

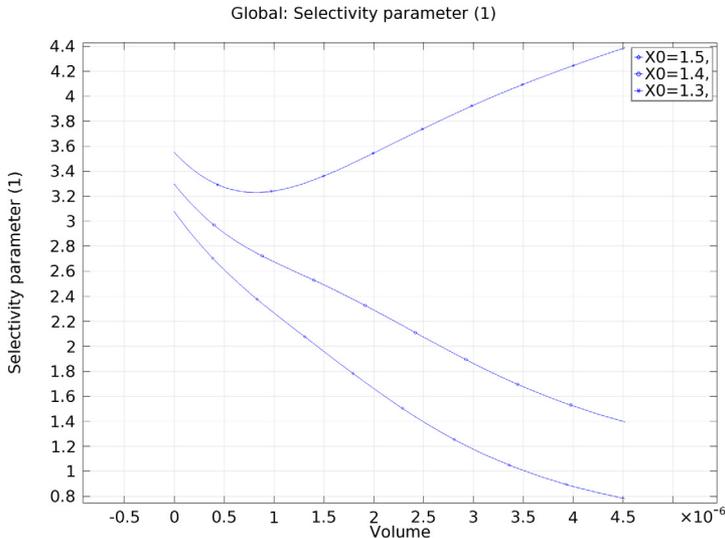
The below figure shows the molar flowrate of NH_3 with respect to the reactor volume the exhaust gas has passed through. What is apparent at the conditions

mentioned above is that a ratio $\text{NH}_3:\text{NO}$ around or above 1.3 is required to ensure that the NH_3 is not completely consumed prior to reaching the reactor's outlet.



Molar flow rate (mol/s) of NH_3 as function of position in the reactive channel.

Going further, three $\text{NH}_3:\text{NO}$ ratios ranging from 1.3 to 1.5 are presented in the next figure along with the selectivity as a function of reactor position. When the $\text{NH}_3:\text{NO}$ ratio is 1.3, the NO reduction is highly prioritized, primarily because NH_3 concentrations become very low.



Selectivity parameter (r_1/r_2) as a function of reactor position.

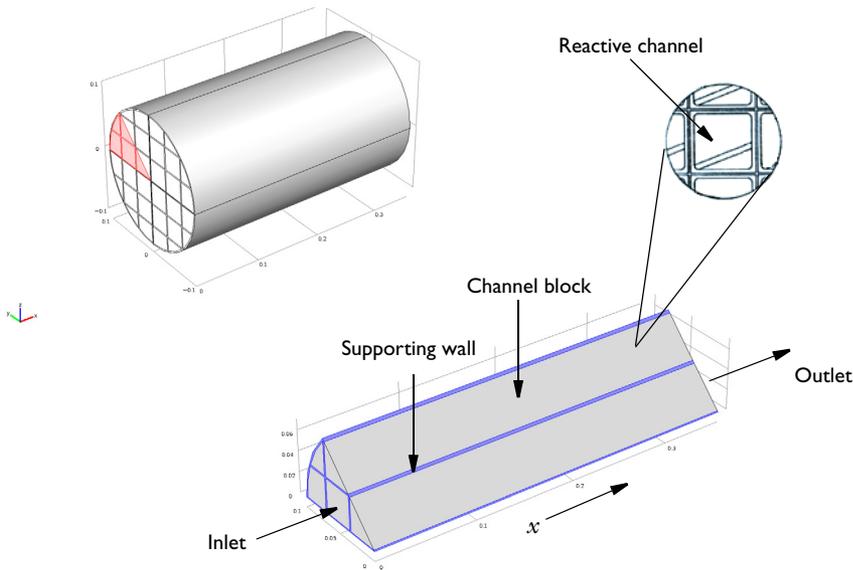
Allowing for some type of operational margin, an $\text{NH}_3:\text{NO}$ ratio of 1.35 is chosen and investigated. This leads to minimal waste of NH_3 without limiting the NO reduction chemistry. Using this figure, conversions of 98.7 % and 97.2 % for both NO and NH_3 consumption are reached, respectively.

Changing the operating temperatures, $\text{NH}_3:\text{NO}$ ratios and other operating parameters by smaller and smaller steps eventually leads to the optimized conditions that grant conversions close to 100% for both reactions. Yet, it should be noted that the catalytic converter is a real reactor with many channels, and the channels differ according to their position in the converter, particularly with respect to heat transferring to the surroundings. So, while the plug-flow reactor model gives a good indication of the monolithic reactor's operation, it certainly does not give the full picture.

Investigating a3D Reactor

The monolith reactor has a modular structure made up of channel blocks coated with the catalytic washcoat, and supported by solid, heat conducting walls. In the

following study, the reactor is 0.36 m long with a 0.1 m radius. Each reactive channel has a cross sectional area of 12.6 mm^2 , and a void fraction of 0.75.



NO reduction chemistry takes place in the channel blocks. Supporting walls hold together the full reactor structure. Symmetry reduces the modeling domain to one eighth of the reactor geometry.

In this study, a pseudo homogeneous approach is used to model the hundreds of channels present in the monolith reactor. As no mass is exchanged between the channels, each is described by a 1D mass transport equation. Furthermore, fully-developed laminar flow is assumed in the channels, such that the average flow field is proportional to the pressure difference across the reactor.

The fluid flow transports mass and energy in the channel direction only. Yet, the energy equation describes not only the temperature of the reacting gas in the channels, but also the conductive heat transfer in the monolith structure and the supporting walls. Heat is conducted through the supporting walls faster than it flows in the channels and monolith structure. Temperature affects not only reaction kinetics but also the density and viscosity of the reacting gas.

Mass Transport

The mass balances describing transport and the reactions in a channel are given by diffusion-convection equations at steady state:

$$\nabla \cdot (-D_i \nabla c_i) + \mathbf{u} \cdot \nabla c_i = R_i \quad (3)$$

Here D_i denotes the diffusion coefficient (m^2/s), c_i is the species concentration (mol/m^3), and \mathbf{u} equals the velocity vector (m/s). The term R_i ($\text{mol}/(\text{m}^3 \cdot \text{s})$) corresponds to the species' rate expression. Mass transport is only allowed in the direction of the channels, corresponding to the x-axis direction in the above 3D geometry.

Fluid Flow

Assuming fully-developed laminar flow in the channels, the average flow field is proportional to the pressure difference across the reactor. On the macro-scale, the monolith can be treated as a porous matrix, with an effective permeability κ (m^2), and modeled using Darcy's Law:

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

$$\mathbf{u} = -\frac{\kappa}{\mu} \nabla p$$

where the density, ρ (kg/m^3), and viscosity, μ ($\text{Pa} \cdot \text{s}$), represent properties of the reacting gas mixture.

Heat Transfer

A single temperature equation describing the heat transfer in the porous monolith reactor can be written, for the stationary case, as

$$\rho_f C_{p_f} \mathbf{u} \cdot \nabla T = \nabla \cdot (k_{\text{eq}} \nabla T) + Q \quad (4)$$

where ρ_f (kg/m^3) is the fluid density, C_{p_f} ($\text{J}/(\text{kg} \cdot \text{K})$) is the fluid heat capacity, and k_{eq} ($\text{W}/(\text{m} \cdot \text{K})$) is the equivalent thermal conductivity. Furthermore, \mathbf{u} (m/s) is the fluid velocity field from above, and Q (W/m^3) is the heat source resulting from the exothermic chemical reactions:

$$Q = Q_1 + Q_2 = -r_1 H_1 - r_2 H_2$$

The equivalent conductivity of the solid-fluid system, k_{eq} , is related to the conductivity of the solid, k_p , and to the conductive of the fluid, k_f , by:

$$k_{\text{eq}} = \Theta_p k_p + \Theta_f k_f$$

where Θ_p denotes the solid material's volume fraction, here 0.25.

Equation 4 is the equation set up by the Heat Transfer interface for a fluid domain. For the supporting walls in the reactor; heat transfer by conduction only applies

$$-\nabla \cdot (k_s \nabla T) = 0$$

where k_s (W/(m·K)) is the thermal conductivity of the solid walls.

Thermodynamic and Transport Properties

As mentioned previously, the temperature affects not only reaction kinetics but also the thermodynamic and physical properties of the reacting gas. Accurate thermodynamic data is required as input to the energy balance equations, both in the plug flow model (Equation 2) and the 3D monolith model (Equation 4). The following set of polynomials are used to describe the species thermodynamic properties:

$$C_{p,i} = R_g(a_1 + a_2T + a_3T^2 + a_4T^3 + a_5T^4)$$

$$h_i = R_g\left(a_1T + \frac{a_2}{2}T^2 + \frac{a_3}{3}T^3 + \frac{a_4}{4}T^4 + \frac{a_5}{5}T^5 + a_6\right)$$

$$s_i = R_g\left(a_1\ln T + a_2T + \frac{a_3}{2}T^2 + \frac{a_4}{3}T^3 + \frac{a_5}{4}T^4 + a_7\right)$$

Here, $C_{p,i}$ denotes the species' heat capacity (J/(mol·K)), T the temperature (K), and R_g the ideal gas constant, 8.314 (J/(mol·K)). Further, h_i is the species' molar enthalpy (J/mol), and s_i represents its molar entropy (J/(mol·K)). A set of seven coefficients per species are taken as input for the polynomials above. The coefficients a_1 through a_5 relate to the species heat capacity, while the coefficient a_6 is associated with the species enthalpy of formation (at 0 K), and the coefficient a_7 comes from the species entropy of formation (at 0 K). The coefficients for these equations are readily available in literature reporting thermodynamic data in the CHEMKIN or NASA formats (Ref. 2, Ref. 3).

In addition to thermodynamic properties, the model equations also require transport properties to accurately describe the space dependent reactor model. For instance, the mass transport (Equation 3) need species specific diffusion coefficients as an input. Kinetic gas theory is used to set up expressions for transport properties such as diffusivities, viscosity, and thermal conductivity as functions of temperature, pressure, and composition. In this example, the species diffusivities (m²/s) are calculated using the formula

$$D = 2.695 \cdot 10^{-3} \cdot \frac{\sqrt{T^3((M_A + M_B)/(2 \cdot 10^3 M_A M_B))}}{P \sigma_A \sigma_B \Omega_D} \quad (5)$$

where Ω_D is a collision integral

$$\Omega_D = f\left(T, \sigma, \frac{\varepsilon}{k_b}, \mu\right)$$

To evaluate Equation 5 you need to specify the characteristic length and energy minimum of the Lennard-Jones interaction potential, that is σ (10^{-10} m) and ε/k_b (K), respectively. The species dipole moment, μ_D (Debye), can also be provided. Each species in the reacting gas has a characteristic set of these constants, and you find their values in the literature, in databases, or from experiments.

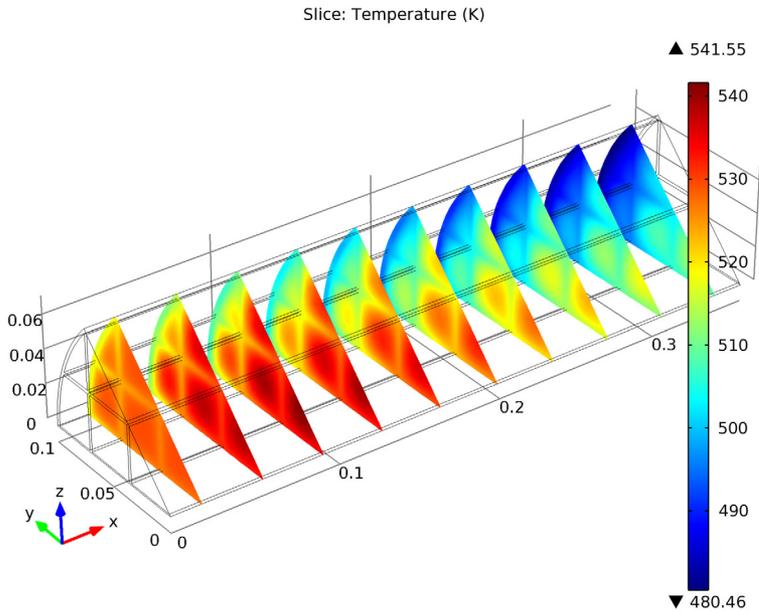
The data parameters used for this model have been compiled from Ref. 4 and are summarized below:

SPECIES	σ [Å]	ε/k_b [K]	μ_D [D]
H2O	809.1	2.640	1.8
N2	71.4	3.798	0.0
NH3	558.3	2.900	1.5
NO	116.7	3.492	0.2
O2	106.7	3.467	0.0

Analysis

The plot below shows the conversion of NO in the monolith channel blocks, where the overall conversion at the outlet is 97.5 %, which is a bit lower than that given in the plug-flow reactor model above. The isosurfaces in the plot show how a channel's

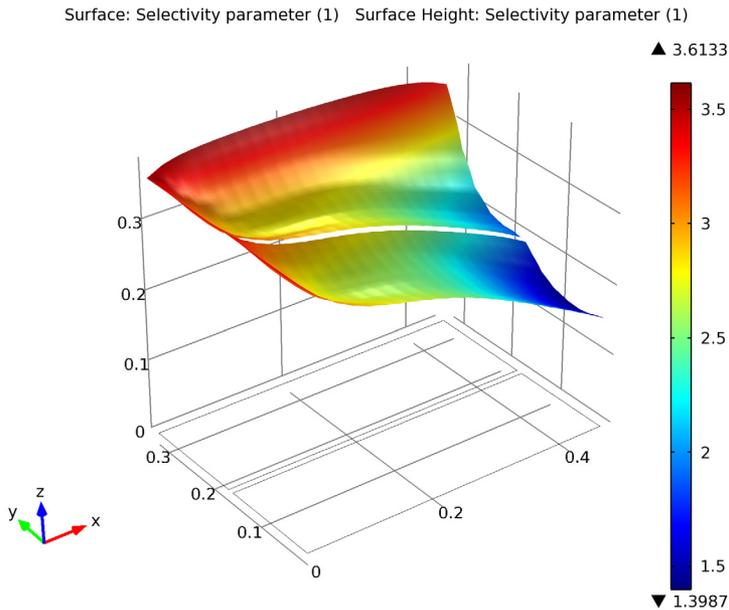
Cross section plots of the reactor temperature are shown below.



Temperature distribution in cross sections of the reactor.

The exothermic reactions increase temperature in the central parts of the reactor, while the temperature is decreased through heat loss to the surroundings. The maximum temperature calculated for the 3D reactor is 541.5 K, which is within the limits found in the perfectly-mixed reactor model above. The effect of the relatively high thermal conductivity of the supporting walls is clearly visible.

A plot of the selectivity on the symmetry surface of the monolith is shown below. The fact that it is greater than 1 throughout indicates that the NO reduction is selectively favored in all regions of the reactor.

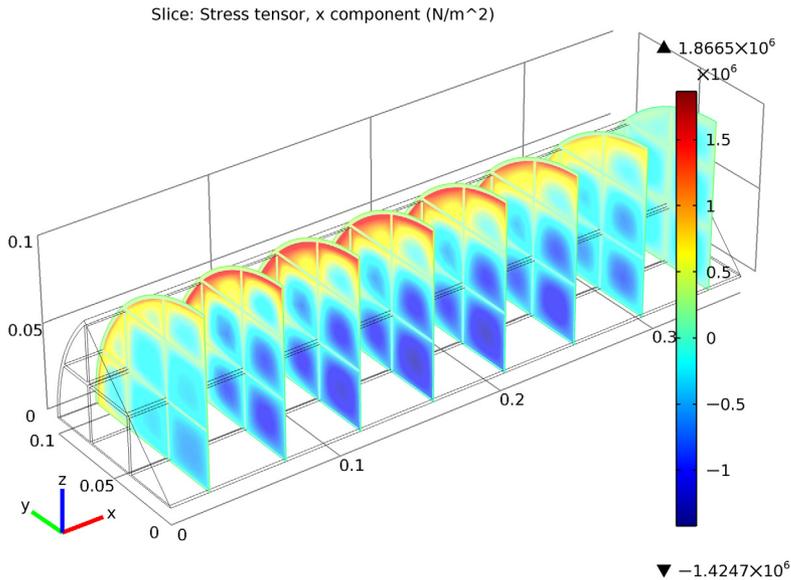


The fact that selectivity is greater than 1 throughout indicates that the desired NO reducing reaction is favored.

The selectivity plot again reveals the space-dependent nature of the problem. Channels in the relatively cold region near the reactor's outer surface display high selectivity throughout, whereas channels in the region close to the center see selectivity falling off comparatively fast. Compared to the single channel model, the 3D reactor shows notably lower values of the selectivity parameter near the center of the outlet. Nevertheless, NO reduction is still favored throughout.

The information from this 3D model can also be used to investigate other aspects of this reacting system. Results can be compared to 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. Alternate catalysts and designs can also be proven.

Even other physical properties, such as the structural integrity of the converter can be investigated, as is shown below.



The stress tensor component in the x direction. Compressive stress is indicated by negative values, and tensile stress by positive values.

References

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3. This example uses data from the GRI-Mech 3.0. <http://www.me.berkeley.edu/gri-mech/>
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Conclusions

Following the strategy described in the beginning of this document has several advantages for studying this catalytic converter. The initial simulations are easy to set up and quite fast to solve. If this reactor was a new design and the chemistry was still being investigated, the simulation results could be compared to experimental results, and the reaction mechanism decided, and kinetic parameters fine-tuned.

Otherwise, the first analysis narrows down process conditions reasonable for the reactor's operation before moving to more advanced and computationally demanding models.

The second analysis provided more information about spatial effects in the reacting system and allowed for a fairly accurate suggestion for operating the reactor to be made. Although a simplified model it was quite easy to set up and fast to solve.

The results from the previous two simulations give a good indication of what the eventual reactor's operating conditions will be. This knowledge helps greatly with setting up a 3D model, which can sometimes be difficult to solve if the input parameters are not close to the eventual solution. And once the model is solved, it provides significant insight into the real converter's operation and design parameters.