

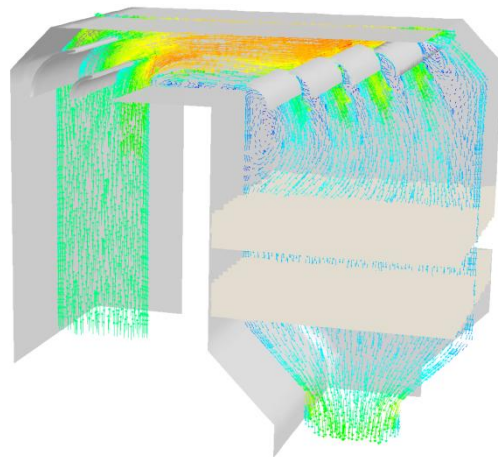
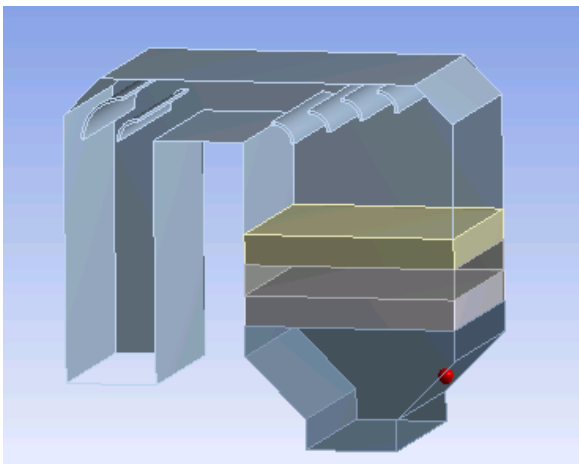
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# Computational Fluid Dynamics for Engineers

## Project 1

### Design of a SCR system for power plant exhaust gas treatment

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This document can be printed and distributed freely in its original and complete form conditioned that it is used as supplementary training material to the book *Computational Fluid Dynamics for Engineers*, Andersson B., Andersson R., Håkansson L., Mortensen M., Sudiyo R., van Wachem B., ISBN 978-1-107-01895-2, published 2011 by Cambridge University Press, The Edinburgh Building, Cambridge CB2 8RU, UK.

Additional resources such as *tutorials, project and lecture notes* are available from the authors and at [www.cambridge.org/9781107018952](http://www.cambridge.org/9781107018952)

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## 1. Project introduction and objectives

Power plants often need to install selective catalytic reduction (SCR) systems to conform to legislation on nitrous oxides (NO<sub>x</sub>) emissions. The SCR system works by injecting ammonia into the flue gas upstream of a fixed monolithic catalyst. Inside the catalyst the NO<sub>x</sub> and ammonia react to produce nitrogen gas and water vapor, thereby reducing the emissions of nitrous oxides. Your task is to design the SCR system.

Critical design parameters include the velocity profile, temperature and ammonia concentration. The SCR system works efficiently only with a uniform velocity and ammonia concentration at the catalyst inlet. Furthermore there is a maximum allowable pressure drop through the SCR system and the ammonia slip is also controlled by legislation.

In Section 1 the problem is described and the objectives are given. All information required to complete the project is given in this section. Section 2 contains the questions related to the project and the instructions on how to prepare the project report. Section 3 contains some tips for Ansys Fluent. However any other CFD software can be used. The reactions occurring in the catalytic layers are already programmed into user defined functions and is available at [www.cambridge.org](http://www.cambridge.org).

The purpose is that you, in accordance with best practice guideline, Chapter 7, design the SCR system. More specific your task is to:

- Specify the dimensions of the catalytic reactor, based on pressure drop considerations only. It is assumed that two layers of catalyst are optimal. The total height of the reactor should be less than 20 m. The inlet and outlets are 6m x 6m.
- Suggest a suitable turbulence model for the reactor (see Table 4.4). Also suggest a discretization scheme for the convective terms.
- Specify the flow regimes (laminar or turbulent) for the different regions of the reactor. Is the flow laminar or turbulent in the monolithic channels?
- Perform a CFD-calculation of the reactor with no reactions. You should be able to almost exactly reproduce the pressure drop from the first task.
- Perform a CFD-calculation assuming perfect mixing at the inlet.
- Choose a strategy for mixing the ammonia with the exhaust. You will have to decide the positions for the ammonia injections to optimize the conversion. The maximum number of ammonia injectors is 20 (You will use symmetry i.e. model one quarter of the reactor so 5 injections will be used).
- Test different temperatures for the full operation (at the same pressure and with homogeneous mixing).
- Calculate the NO<sub>x</sub> conversion and the ammonia slip for each production case.
- Write a technical report in English. Assume that the report will be read by people who have experience in CFD, but no experience in SCR systems.
- Give an oral presentation in English. Recommended 15 min review of your project results + 5 min for questions. The presentation should be prepared for an audience that is not acquainted with the SCR system, but have experience in CFD. You should be prepared to answer questions from the audience.
- Read the project report written by another group and ask relevant questions.

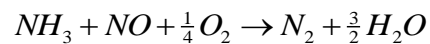
### 1.1 Project prerequisites

It is recommended that you have read Chapters 1-7 in the book *Computational Fluid Dynamics for Engineers* and you must have completed the three tutorials. Regardless of what CFD software you use, you will find all required data in Section 1. Instructions related to the project report is found in Section 2.

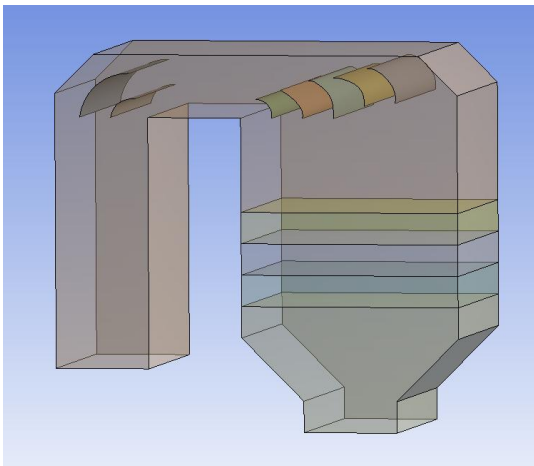
If you use Ansys Workbench you should read Section 3 in this manual to get some tips on how to setup the model. If you use any other CFD software you should use the data given in Section 1 and use the software documentation.

### 1.2 Project problem description

The purpose of this project is to design a SCR system and evaluate its performance through CFD simulations of the reactions that occur within the monolithic catalyst. Nitrogen oxides, NO<sub>x</sub> (NO+NO<sub>2</sub>), is formed in combustion with air at high temperatures. Nitrogen oxides are toxic and contributes to acidification of the landscape and must be removed. The most common process is selective catalytic reduction, SCR, using ammonia.

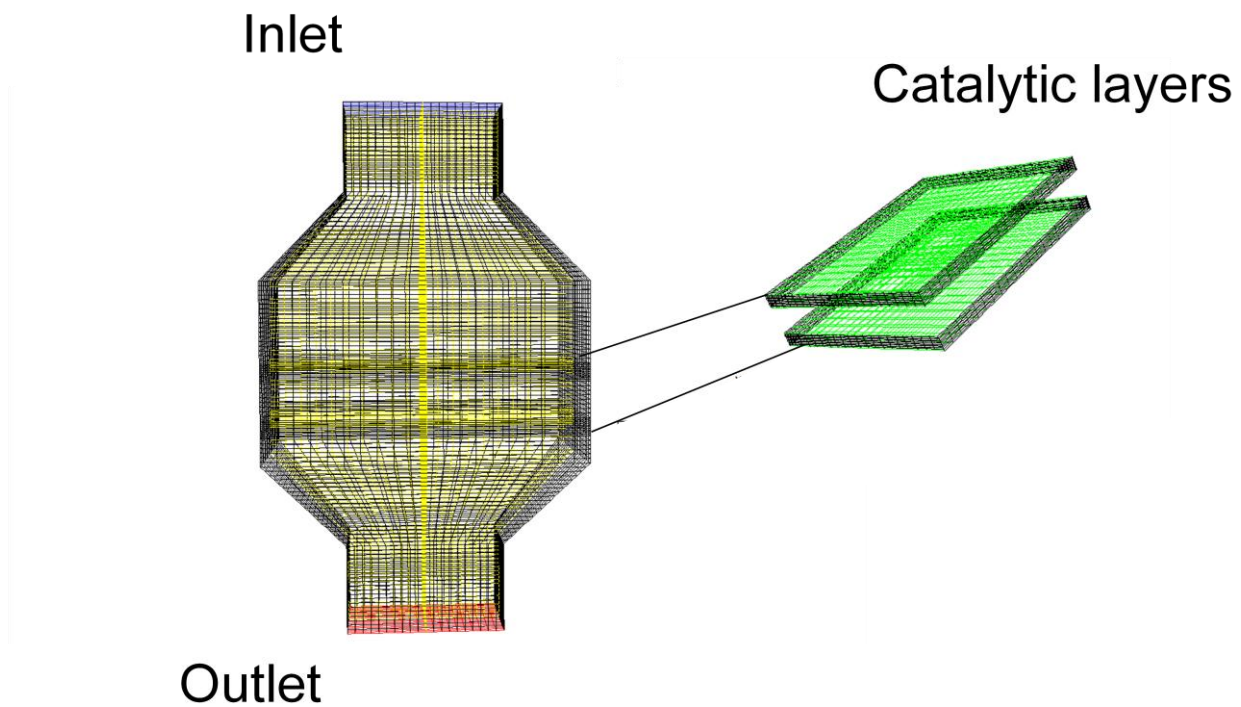


The SCR system considered in this project is shown in Figure 1. The reactor should have a capacity to remove a major part of the NO<sub>x</sub> emission at full production in the power plant.



**Figure 1.** Schematic overview of a SCR reactor.

Due to computational time you will model a simplified SCR system without evaporation of the spray and without the flow in the U-turn. Thereby you will be able to use symmetry and model only one quarter of the SCR system as shown in Figure 2.



**Figure 2.** Schematic view of a simplified SCR reactor.

The power plant is run when the demand for electrical power is high. During a normal year the plant is run according to Table 1.

**Table 1.** Normal year production.

% of full production	Days
100	26
75	4
50	3
25	1
0	331

At full production the power plant produces **250 MW** of electricity. The exhaust conditions at the reactor inlet are shown in Table 2.

**Table 2.** Exhaust conditions (for volumetric flow rate  $N = 1$  bar, 293 K).

% of full production	25	50	75	100
Flow $\text{Nm}^3/\text{h}$	206 000	356 000	493 000	683 000
Temperature $^{\circ}\text{C}$	290	310	340	365
Pressure Pa	99 650	99 400	99 000	98 400
Mole fraction of NO	$3.8 \cdot 10^{-4}$	$4.2 \cdot 10^{-4}$	$4.8 \cdot 10^{-4}$	$4.9 \cdot 10^{-4}$
Mole fraction of $\text{H}_2\text{O}$	0.125	0.125	0.125	0.125
Mole fraction of $\text{O}_2$ and $\text{CO}_2$	0.0625	0.0625	0.0625	0.0625

Nitrogen,  $\text{N}_2$  is the bulk of the exhaust flow.

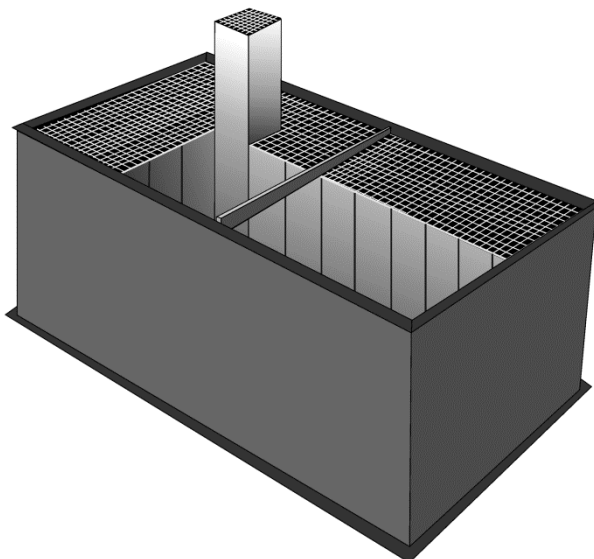
Ammonia is mixed with NO through some simple injection device that you design. The ammonia slip (unreacted ammonia leaving the reactor) must never exceed **15 ppm**. The reactor should be designed for a pressure-drop of no more than **600 Pa** over the catalytic layers at full operation. The catalyst is a monolith that consists of many straight squared channels as shown in Figure 3.

## Technical data -SCR system

### Catalyst module information

The catalytic reactor is a monolith that is manufactured by extruding the catalytic material. The catalytic material is 1.5%  $V_2O_5$  and 9%  $WO_3$  on  $TiO_2$  (use Dolomite). The elements are mounted in modules of steel as shown in Figure 3. One module consists of 72 elements. Each element consists of 625 square channels (5mm).

Density of catalyst material:	1770	$kg/m^3$
Specific area of catalyst material:	88	$m^2/g$
Pore size:	250	$\text{\AA}$
Number of acidic sites:	$3.48 \cdot 10^{18}$	$m^{-2}$
Dimensions of catalyst element:	150 x 150 x <b>750</b>	mm
Number of cell openings per element:	25 x 25	
Size of cell opening:	5.0 x 5.0	mm
Number of elements in module:	6 x 12	
Size of module:	1900 x 960 x <b>1050</b>	mm



**Figure 3.** Catalyst module partly filled with elements.

## Physical constants and relationships

The following parameters are contained in the user defined functions for the reaction rate in the catalytic layers.

### Molecular diffusivities in the mixture:

$$D_{\text{NO}} = 1.14 \cdot 10^{-9} \cdot T^{1.75} \text{ m}^2/\text{s}$$

$$D_{\text{NH}_3} = 1.07 \cdot 10^{-9} \cdot T^{1.75} \text{ m}^2/\text{s}$$

$$D_{\text{O}_2} = D_{\text{N}_2} = D_{\text{CO}_2} = D_{\text{H}_2\text{O}} = 1.1 \cdot 10^{-9} \cdot T^{1.75} \text{ m}^2/\text{s} \text{ (Approximated as equal)}$$

### Pore diffusivity:

The diffusivity within the porous catalyst walls is much lower than in the gas bulk, and the effective pore diffusivity is given by:

$$D_{\text{eff}} = 7.68 \cdot 10^{-8} \cdot T^{0.6} \text{ m}^2/\text{s} \quad \text{(Approximated equal for all components)}$$

### Viscosity:

$$\mu = 1.23 \cdot 10^{-6} \cdot T^{0.6} \text{ Pas} \quad \text{(Mixture)}$$



## Pressure drop

The pressure drop is a function of the velocity in the monolith channels and thus a function of the number of modules in each layer. Use this and the given recommended pressure drop to estimate the dimensions of the reactor.

Arrange the modules in rectangular layers

- 2 catalyst layers
- X modules per layer
- 72 elements per module
- 625 channels per element

Find X from the pressure drop,  $\Delta P = 600 \text{ Pa}$  → channel velocity → x number of modules

**Poiseuille equation:**

$$\Delta P = \frac{32\mu Lv}{d^2}$$

where L is the height of the catalyst layers ( $2 \times 0.75 \text{ m}$ ), v is the average gas velocity inside each channel and d is the width of a channel.

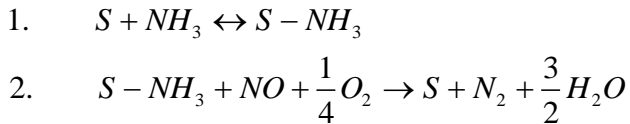
Specify parameters in the software pressure drop model for porous material (for Fluent see guidelines in Section 3). You should be able to reproduce the pressure drop. Get a good starting guess and then adjust it.

Note that the permeability is high along the channels and very low cross the channels.

## Mass transfer and reactions

The reaction rates and mass transfer are given in the udf SCR.C.

### Reactions:



Where S is an active site.

At steady state conditions there is a balance in the porous catalyst.

$$\left\{ \begin{array}{c} \text{Adsorption} \\ \text{of } NH_3 \end{array} \right\} - \left\{ \begin{array}{c} \text{Desorption} \\ \text{of } NH_3 \end{array} \right\} - \left\{ \begin{array}{c} \text{Consumed } NH_3 \\ \text{by reaction} \end{array} \right\} = 0$$

$$r_{1+} - r_{1-} - r_2 = 0$$

where

$$r_{1+} = k_{1+} c_{NH_3} (1 - \theta_{NH_3})$$

$$r_{1-} = k_{1-} \theta_{NH_3}$$

$$r_2 = k_2 c_{NO} \theta_{NH_3}$$

Here  $r$  is the *reaction rate in molecules per active site and second*,  $c$  is the concentration in mole/m<sup>3</sup> and  $\theta_{NH_3}$  is the fractional coverage of  $NH_3$  on the active sites.  $k$  is the rate constant given by the Arrhenius expression:

Which gives an expression for the coverage of  $NH_3$ .

$$\theta_{NH_3} = \frac{k_{1+} \cdot c_{NH_3}}{k_{1-} + k_{1+} \cdot c_{NH_3} + k_2 \cdot c_{NO}}$$

Inserted into the rate expression for  $r_2$  one gets

$$r_2 = \frac{k_2 \cdot K \cdot c_{NO} \cdot c_{NH_3}}{1 + K \cdot c_{NH_3} + \frac{k_2}{k_{1-}} \cdot c_{NO}}$$

where  $r_2$  is the rate of consumption of ammonia. The reaction rates of the other components are given from stoichiometry.

The rate constants are given by

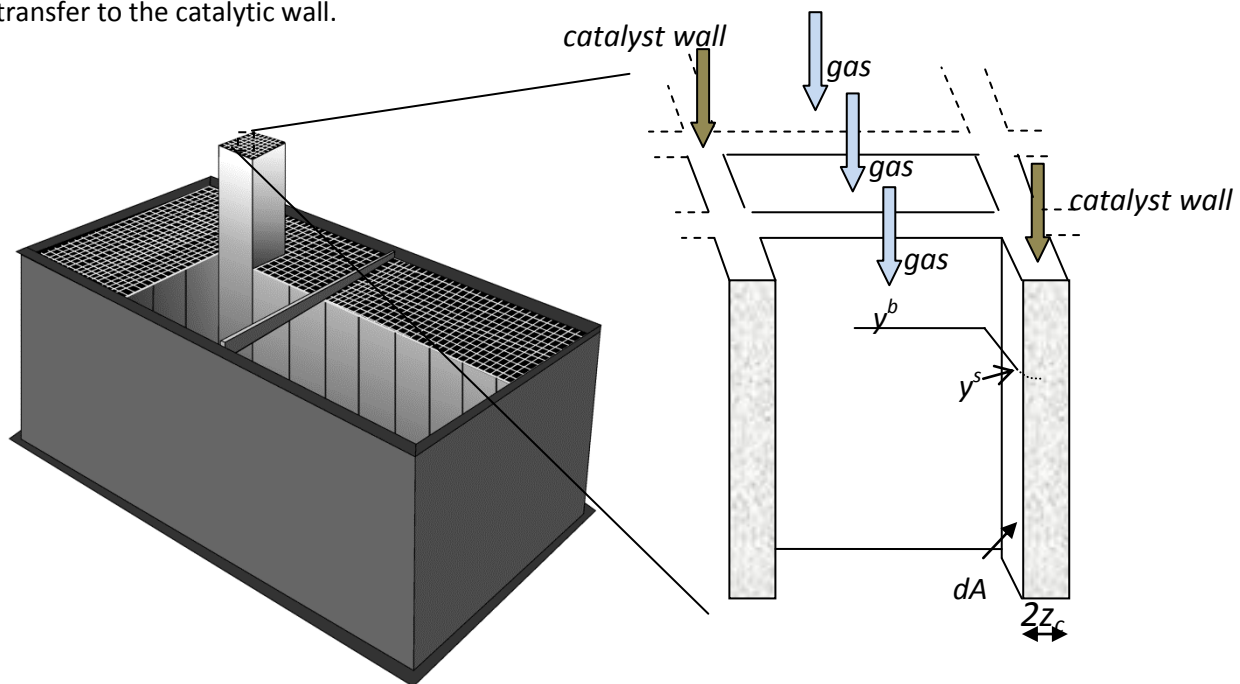
$$k_i = A_i e^{-\frac{E_i}{RT}} \quad K = \frac{k_{1+}}{k_{1-}}$$

**Kinetic parameters:**

Reaction No.	$A_{i+}$	$E_{i+}$ (kJ/mole)	$A_{i-}$	$E_{i-}$ (kJ/mole)
1	0.614	0	$1.99 \cdot 10^5$	98
2	$8.39 \cdot 10^5$	59.5	-	-

$A_i$  is the pre-exponential factor and  $E_i$  is the activation energy for reaction  $i$ . + denotes forward reaction and - denotes backward reaction.

Reactions occur inside the catalyst walls of the catalytic elements, as shown in the Figure below. Here  $y^b$  is the molar fraction in the bulk and  $y^s$  the molar fraction at the surface. These walls are far too small to be fully resolved in a CFD-calculation (it would require an enormous amount of calculation cells) and *a different strategy than in Tutorial 1 is thus needed*. In this project we make the assumption that at steady state there is a balance in each computational cell between reaction in the catalytic wall and mass transfer to the catalytic wall.



To calculate the reaction in the catalytic walls we utilize the effectiveness factor that is given by the inverse of the Thiele modulus. Hence the reaction rate is found from the following correlations:

Balance of mass transfer and reaction rate:

$$\left\{ \begin{array}{c} \text{Mass transfer} \\ \text{through} \\ \text{gas film} \end{array} \right\} = \left\{ \begin{array}{c} \text{Reaction rate} \\ \text{inside} \\ \text{catalyst} \end{array} \right\}$$

$$k_c \cdot C_{tot} (y^b - y^s) \cdot dA = rx \cdot \eta \cdot dw$$

where  $k_c$  is the mass transfer coefficient,  $y$  the molar fraction in the bulk and at the surface,  $\eta$  is the effectiveness factor and the infinitesimal catalytic element is given from geometrical relations by

$$dw = \rho \cdot z_c \cdot dA$$

where  $\rho$  is the density of the catalyst,  $z_c$  is the half-width of the catalyst walls and  $dA$  is an infinitesimal area of the catalyst wall.

Together the two equations give

$$k_c \cdot C_{tot} (y^b - y^s) - rx \cdot \eta \cdot \rho \cdot z_c = 0$$

Thiele modulus:

$$\phi = \frac{z_c \cdot rx(C^s)}{\sqrt{2}} \left[ \int_0^{C^s} D_{eff} \cdot rx \cdot d\alpha \right]^{-1/2}$$

These equations are solved for each computational cell in the catalytic layers for each iteration.

The mass transfer coefficient  $k_c$  is estimated from the Sherwood number  $k_c = Sh \cdot D / d$  and the Sherwood number is a function of Reynolds number and the Length of the channel

$$Sh = 3.53e^{0.0298 Re \frac{d}{L} Sc}$$

The Sherwood number is used in the UDF to find the mass transfer coefficients for transport of NO, NH<sub>3</sub> and O<sub>2</sub> from the fluid in the open channels to the catalytic walls. Read the UDF file to understand what it calculates. Give a short description in your report.

## 2. Project report instructions

### Minimum requirements on report in SCR project

The report is a part of the examination of the course. Make sure that your simulation follows the recommendations in “Best Practice Guidelines”, Chapter 7 in the textbook. The theory and simulation sections should account for roughly half of the overall project report. Ensure that you have addressed all objectives given in Section 1. All results and figures must be commented. You should particularly comment if the results are expected or not. More importantly you should explain how the results are connected to the SCR system performance. In order to be approved the project report should at least contain the following:

### Summary

**Introduction**                      Problem statement and objective

**Theory**

All the governing equations solved in the CFD simulations and the eq. for the pressure drop. Include a section on how the dimensions of the reactor were calculated.

**Simulation**

Discuss your simulation e.g. what did you model, what settings, assumptions, boundary conditions, initial conditions, etc.

**Tabular Results**

Reactor dimensions (number modules per layer and arrangement in the layers)

Dosage of ammonia (all production cases)

NO<sub>x</sub> reduction (all production cases)

Ammonia slip (all production cases)

Pressure drop (all production cases)

## CFD-results

Absolute pressure (full production)  
Velocity vectors (full production)

## Discussion

Is the solution grid independent?  
Are the requirements for wall functions fulfilled?  
Is your choice of inlet conditions important for the reactor performance?  
Is the solution dependent on the turbulence model or the discretization schemes?

Discuss the effects of mixing and temperature on conversion. Is it mixing or kinetics that mainly limits the conversion? Discuss if you think the SCR-reactor can be accurately predicted with a 2D mesh.

## Conclusions

## Optional tasks

Discuss simulation methods to solve the problem using either  
1.) injection of liquid spray for ammonia droplets  
2.) injection of gaseous ammonia that reacts with NO at high temperature without a catalyst.

Perform simulations using the proposed method.

## Information for Chalmers students:

For your convenience we have suggested a schedule.

### Week 1 (the week you start the project)

- Introduction
- Calculate the dimensions of the reactor
- Design the reactor and generate the mesh
- Reproduce the pressure drop in FLUENT

### Week 2

- Investigate the reactor design and evaluate mixing

### Week 3

- Run simulations for all cases and finalize the project report. The report is a very important part of the project. A good report will count more than 'correct' calculations.

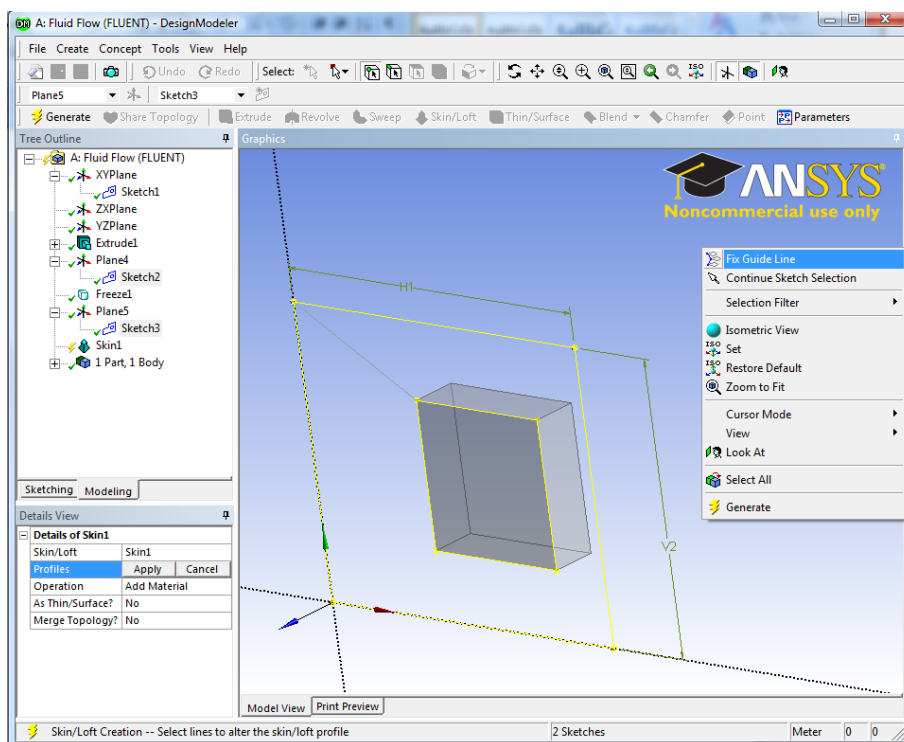
Turn in your report on time, the reports will not be accepted if they are late thus resulting in not passing the project.

### 3. Tips (Ansys Workbench)

This sections contains selected tips and is not intended as complete instruction on how to generate the CAD model and mesh. It also contains instruction on how to compile and load the UDF library which has not been shown in the tutorials.

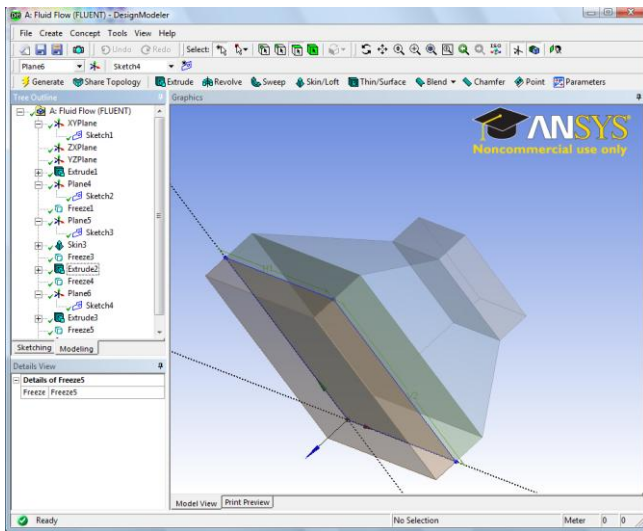
#### Geometry

1. **Draw** the first rectangle (3m x 3m) in XY plane. **Extrude** a suitable length Z1. **Freeze**
2. **Create a new plane** Z1 from the origin. **Generate**.
3. **Draw** a new rectangle (3m x 3m). **Generate**
4. **Create a new plane** Z2 from the origin. **Generate**.
5. **Draw** a new rectangle with the dimensions you calculated( $X_m \times Y_m$ ). **Generate**
6. In modeling select the two last rectangles (Sketch2 and CTRL Sketch3).
7. Click **Skin/Loft**. There will be a line connecting two corners. If the line does not connect the right corners, right click and select **Fix Guide Line**. You can now move the line. When the right corners are selected select **Generate**. **Freeze**



Create **new planes** and **draw** new rectangles on the planes. Use **Extrude** when the XY dimensions are not changing and **Skin/Loft** when they change. **Do not forget to Freeze** after each volume.

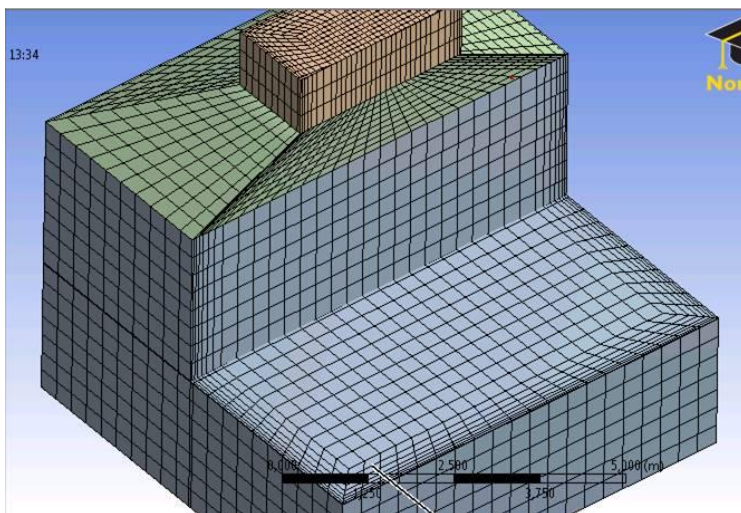




## Meshing

You should preferably use a hexahedral mesh, it makes it easier to reach convergence. Avoid using tetrahedral mesh. You can for example use mesh controls for multizone -mapped mesh method hexa, and use mesh controls for inflations. This produces a mesh as shown in the figure below. You can use symmetry and mesh one quarter of the system to reduced the computational time.

Hint use both 'single select' and 'box select' to efficiently select all volumes and surfaces.



## Fluent

You will use a UDF (c-file), 'SCR.c', which calculates the reaction rates in the monoliths including the mass transfer rate.

When you run your simulations with reactions you have to specify **two** User Defined Memories (UDM).

### Define\User-Defined\Memory

The difference between interpreted and compiled UDFs is more than a factor 3 in simulation time for this particular code. Hence, you have to compile the UDF to save computational time. Compilation requires that you have a compiler installed.

### Define\User-Defined\Functions\Compiled

add source file (select SCR.c)

build library

load library

A text like this should appear in the text user interface.

Opening library "libudf"...

Library "libudf\win64\3ddp\libudf.dll" opened

NH3\_rxrate

NO\_rxrate

O2\_rxrate

CO2\_rxrate

H2O\_rxrate

N2\_rxrate

D\_mix

viscosity

Note that the library must be compiled for the particular operating system, in this case win64 folder tells that compilation is done for Windows 64 bit version.

You should now be able to set the diffusivity and viscosity of the mixture and set the source terms inside your catalysts.

The molecular and the effective diffusivities are included in the UDF 'D\_eff' and must be enabled in FLUENT.

The viscosity is included in the UDF called 'viscosity' and must be enabled in FLUENT

The pressure drop in the catalytic layers is given by the Poiseuille equation and is NOT calculated in a UDF.

The species must be defined in the following order: NH<sub>3</sub>, NO, H<sub>2</sub>O, O<sub>2</sub>, CO<sub>2</sub>, N<sub>2</sub>. The UDF assumes this order.

All species source terms must be enabled in Fluent. These are programmed into the SCR.c file.

For injection of NH<sub>3</sub> you will need to separate the inlet into smaller parts. To be able to do separations, mark cells in the 'Adaption-Region' panel and separate fluid zones in 'Grid-separate-Face'. Both ammonia and exhaust gas will flow through these surfaces.

One of the first steps is to determine the porous bed parameters based on your calculate pressure drop. Porous media are modeled by the addition of a momentum source term to the standard fluid flow equations. The source term is composed of two parts, a viscous loss term (the first term on the right-hand side in the equation below) , and an inertial loss term (the second term on the right-hand side):

$$S_i = - \left( \sum_{j=1}^3 D_{ij} \mu v_j + \sum_{j=1}^3 C_{ij} \frac{1}{2} \rho |v_j| v_j \right)$$

here  $S_i$  is the source term for the  $i$ th (  $x$ ,  $y$ , or  $z$ ) momentum equation, and  $D$  and  $C$  are prescribed matrices. This momentum sink contributes to the pressure gradient in the porous cell, creating a pressure drop that is proportional to the fluid velocity (or velocity squared) in the cell. Compare this equation with the Poiseuille equation and set  $D_{ij}$  (and maybe  $C_{ij}$ ) accordingly. Note that the permeability is high along the channels and very low cross the channels.

NOTE The pressure drop in the catalytic layers is given by the Poiseuille equation and is NOT calculated in a UDF. To include the effect of the multiple channels one must divide the Poiseuille equation with the fraction of channel-volume to total volume in the catalyst layers.

## Judging convergence

Note that reaching convergence under all conditions is not easy in this project. Your simulations can take an entire day to finish iterating in some situations. However, we must stress the importance of convergence in this case. In designing a SCR system the  $\text{NO}_x$  must be converted, but it is equally important to prevent any ammonia slip. Thus, you will need to modify the default settings for the residuals.

Convergence is best evaluated by monitoring the NO and  $\text{NH}_3$  molar fraction in the outflow. These molar fractions should be stable and the reacted NO should be equal to the reacted  $\text{NH}_3$ .