Mathematical Modeling in Chemical Engineering

Model formulation, simplification and validation

Tutorial 1 - 6

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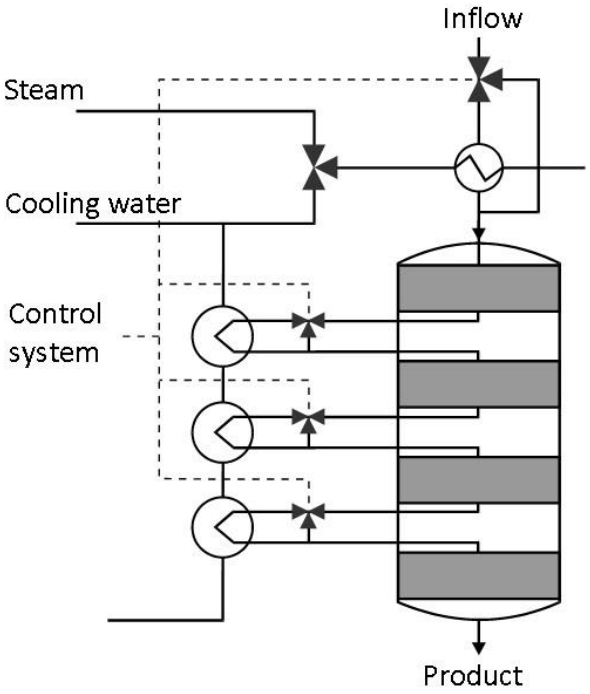
1. Tutorial introduction and objectives

In this tutorial a solid-bed-reactor used for hydrogenation of acetylene is studied. Tutorial 1-5 deal with model formulation and simplification. Tutorial 6 deals with statistical analysis of the model.

The purpose is that you learn how to:

- Construct mathematical models by formulating balance equations.
- Solve the equations by using the attached Matlab files.
- Perform regression analysis.
- Validate the model and assess the individual model parameters.

A slip of maximum 5 ppm acetylene is accepted from the reactor. The reactor consists of four beds connected in series with cooling in between, as shown in the figure below. The inflow could either be pre-heated or cooled before entering the reactor.



The following reactions occur inside the reactor:

$C_2H_2 + H_2 \rightarrow C_2H_4$ (1)
$C_2H_4 + H_2 \rightarrow C_2H_6$ (2)
C_3H_4-ma $+ H_2 \rightarrow C_3H_6$ (3)
C_3H_4-pd $+ H_2 \rightarrow C_3H_6$ (4)

At start up, after regeneration of the catalytic beds, the temperature in the bed could rise above 400 ^oC if the catalytic activity in the bed is high and if the temperature at the inflow is unsuitable. Cooling of the bed is then needed to control the reactor. A new method where nitrogen gas is used as inflow to cool down the bed is therefore of interest to study. In the following tutorial balance equations describing the heat and mass transport in the reactor should be derived and used to understand how the reactor works and how it can be successfully operated.

2. Tutorial prerequisites

It is recommended that you have read the text book (*Mathematical Modeling in Chemical Engineering*), particularly the chapters about model formulation and simplification before you solve Tutorial 1-5. Before you start with Tutorial 6 you should have studied Chapter 7 about model validation and learned how to perform statistical analysis of mathematical models.

3. Tutorial instruction

To investigate the impact of changing parameters the attached MATLAB program could be used. All data needed for the analysis is included in the attached Matlab files. These files can be downloaded from the publisher at *www.cambridge.org/rasmuson*. Run the Matlab m-file "start_file.m" and follow the instructions to study reactor performance, based on the balance equations derived in tutorial 1-5. Run the m-file "call_func.m" to complete tutorial 6. Make sure you have write permission in the folder where you place the Matlab-files. On some computer systems you need to modify the 'save' command in the Matlab-files and explicitly define the folder where the files should be saved, i.e. save 'constants.mat' can be replaced by save 'D:\constants.mat'.

3.1 Tutorial 1

Write down and simplify the transient heat and mass balances describing the reaction in the reactor when it is assumed to be adiabatic. Discuss how the transient temperature and concentration profiles in the reactor will look like during start up from 60^{o}C. How will the profiles change if the start up temperature is increased? At stationary conditions the temperature in the reactor is preferably 90^{o}C. If the balances are solved at stationary conditions why do the profiles change in comparison to the transient case? What will happen if the amount of acetylene in the inflow is increased?

3.2 Tutorial 2

Rework tutorial 1 when the reactor is assumed to be non-adiabatic and the outdoor temperature is -10 ^{o}C and the wind speed is 20 m/s. What will happen if the wind speed or the outdoor temperature changes? Discuss the effect of increasing the wall thickness or changing the flow rate inside the reactor.

3.3 Tutorial 3

Derive the mass and heat balances over the reactor including the axial and radial dispersion. Use Ficks and Fouriers laws to describe the axial dispersion. What boundary conditions should be used? What will be the effect if the particle diameter or the porosity changes?

3.4 Tutorial 4

Write down and simplify balances describing the transport of mass and heat inside a catalytic particle. What will happen if the diameter or porosity of the particle is changed? To further investigate the reaction the transport of reactants from the bulk through the film and pores in the catalytic material as well as diffusion inside the catalytic material to the active sites can be studied. Determine where the main resistance is found.

3.5 Tutorial 5

Rework tutorial 1 for the case when the reactor is cooled down with nitrogen gas at a temperature of 0 ^{o}C. Use a flow rate of nitrogen gas which gives a maximum pressure drop over the reactor of 1 bar. What will the transient temperature profiles inside the bed and in the gas stream look like? Assume that the gas flow is a plug flow, the temperature gradients inside the catalytic particles could be neglected and that

the temperature profile in the bed is stationary. What will be the difference if the nitrogen gas is added in the same direction as the feed or in a counter-current direction?

3.6 Tutorial 6

Hydrogenation of ethene to ethane occur in a differential reactor with a catalyst made of cobalt-molybdenum

$$\underset{(H)}{H_2} + \underset{(E)}{C_2H_4} \rightarrow \underset{(EA)}{C_2H_6}$$

Measurement data is found in the Table below:

Case	Reaction rate Mol/(kg cat·s)	P_E bar	P_{EA} bar	P_H bar
1	1.04	1	1	1
2	3.13	1	1	3
3	5.21	1	1	5
4	3.82	3	1	3
5	4.19	5	1	3
6	2.391	0.5	1	3
7	3.867	0.5	0.5	5
8	2.199	0.5	3	3
9	0.75	0.5	5	1

The following rate expressions have been suggested:

a. $$r = \frac{k P_E P_H}{1 + K_{EA} P_{EA} + K_E P_E}$$

b. $$r = \frac{k P_E P_H}{1 + K_E P_E}$$

c. $$r = \frac{k P_E P_H}{(1 + K_E P_E)^2}$$

d. $$r = k P_E^a P_H^b$$

For each rate expression:

1. Determine the parameters.
2. Determine the 95% confidence interval and the correlation between each parameter.
3. Investigate the parameter significance.
4. Do a residual analysis.
5. Use the results to determine which model that best describes the measurement data.