Introduction to Reactor Design, 3K4
Course project

Kevin Dunn, kevin.dunn@mcmaster.ca **Due: 04 April 2013**

Project objectives:

- To demonstrate your understanding of designing a packed bed reactor.
- Show that you can calculate the required design taking heat, pressure drop and changing physical properties into account.
- Design and create a plan of action that you will follow to achieve your goal.
- To reflect afterwards on your group's progress and judge how you followed your plan.

You are required to design a shell and tube packed-bed reactor for methanol synthesis. The complete problem statement follows.

1. Projects are to be tackled in groups of 3, with one report per group. Each student will submit at the end of the project a confidential assessment of the relative contributions of the members of the group.
2. The methodology used in the design of the reactor must be clearly explained; all assumptions must be identified and evaluated; the results must be clearly presented and discussed. In particular you *must* have a section at the start of your report where you: "**clearly explain the strategy you will follow to achieve the project's objective**". Use bullet points showing the sequence of steps you planned.
3. Reports must be written in an acceptable and professional style and should not exceed 15 typed pages (*including* any appendices). Any code you choose to include in part of your page limit. You must submit your report using Google Docs. More details to come on the course website.
4. All published information consulted must be appropriately referenced.
5. At the end you must have a section called "**Reflection**". Answer these 3 questions in the section:
   (a) How accurately did our group stick to the plan (there is no penalty from deviating from your plan, but describe why you deviated).
   (b) How would we go about the project differently if we could redo it?
   (c) What did we learn from doing this project (bullet points are OK).

Problem statement

A new catalyst has been proposed for the synthesis of methanol from carbon monoxide and hydrogen gas. This catalyst is reasonably active between temperatures of 330 K to about 430 K. The reactions to be considered are:

$$\mathrm{CO} + 2\mathrm{H_2} \rightleftharpoons \mathrm{CH_3OH}$$
$$\mathrm{CO} + \mathrm{H_2O} \rightleftharpoons \mathrm{CO_2} + \mathrm{H_2}$$

The reactions are elementary and occur in a reactor containing tubes packed with a precious metal catalyst on a silica support. Heat is removed from the reactor by generating steam on the shell side of the tubes. The feed consists of $\frac{7}{15}$ hydrogen gas, $\frac{1}{5}$ carbon monoxide, $\frac{1}{5}$ carbon dioxide, and $\frac{2}{15}$ steam. The total flow rate is $300\,\mathrm{mol.s^{-1}}$. The entering pressure may be varied between 1 atm and 160 atm and the entering temperature between 300 K and 400 K. A total tubular rector volume of $2\,\mathrm{m^3}$ is to be used.

The following tasks should be completed:

1. Discuss the commercial application of this reaction in terms of the overall process, economics, process conditions, reactor types and configurations typically used, type of catalyst, typical conversion and end product usage.

2. Assuming isothermal and isobaric conditions, determine the entering conditions of temperature and pressure that will optimize the production of methanol. *Hint*: Do this by conducting several simulations at discrete combinations of T_0 and P_0.

3. Carry out a detailed reactor design of a shell and tube reactor for the optimal feed conditions determined in part 2. Pressure drop and non-isothermal effects are to be taken into account. The shell side temperature can be controlled by adjusting the steam pressure, and may be assumed constant at a value specified by you. Physical property estimation sources, techniques and assumptions should be clearly presented. The design should include the following:

   - the reactor dimensions and number of tubes
   - the reactor conditions; including composition, pressure and temperature profiles (as a function of reactor length).
   - **Not required**: mechanical design of the reactor, including specification of the reactor material of construction, shell and tube wall thickness and capital cost for the design. A mechanical sketch of the reactor should be included.

4. Determine the effect of variations in:

   - ratio of feed H_2 to CO,
   - ratio of feed H_2O to CO,
   - assumed heat transfer coefficient, U

   on the rate of methanol production in your reactor by varying each of the parameters by $\pm 10\%$. Tabulate the results against the conditions for the nominal design and discuss the significance of these results on your design. Bonus grades will be awarded for clear, graphical visualizations of the sensitivity analysis.

5. All results must be presented in SI units throughout the report.

Additional problem information

Thermodynamic and rate data

T is in Kelvin, but $R = 1.987\,\text{cal.mol}^{-1}.\text{K}^{-1}$. The subscript 1 refers to the methanol reaction, while subscript 2 refers to the water-gas shift reaction.

$$K_{C,1} = 131667(0.001987T)^2\ \exp\left[\frac{30620}{R}\left(\frac{1}{T}-\frac{1}{298}\right)\right] \qquad \left[\frac{\text{dm}^3}{\text{mol}}\right]^2$$

$$K_{C,2} = 103943\ \exp\left[\frac{9834}{R}\left(\frac{1}{T}-\frac{1}{298}\right)\right] \qquad [-]$$

Updated: $$k_1 = 0.933\times10^{-6}\ \exp\left[2.5\left(\frac{31400}{R}\left(\frac{1}{330}-\frac{1}{T}\right)\right)\right] \qquad \left[\left(\frac{\text{dm}^3}{\text{mol}}\right)^2 \text{s}^{-1}\right]$$

Updated: $$k_2 = 0.636\times10^{-6}\ \exp\left[\frac{18000}{R}\left(\frac{1}{300}-\frac{1}{T}\right)\right] \qquad \left[\frac{\text{dm}^3}{\text{mol}\cdot\text{s}}\right]$$

Reactor equipment data

- Catalyst bed void fraction: 40%
- Catalyst density: $1600\,\text{kg.m}^{-3}$
- Tube diameter (i.d.): 3.81 cm

Updated/new values below:

- Overall heat transfer coefficient: $631\,\text{W.m}^{-1}.\text{K}^{-1}$
- Tube diameter (o.d.): 4.20 cm
- Shell side water temperature: 373 K
- Catalyst particle size: 5mm
- Average gas viscosity, assumed constant over all temperature: $7.5\times10^{-6}\,\text{Pa.s}$
- Number of tubes in the heat exchanger: 250 tubes

Additional literature resources

The following potentially useful resources exist:

- Seider, W.D., J.D. Seader and D.R. Lewin, *Product and Process Design Principles*. 2nd Ed., `TP 155.7.S423 2004`
- Peters and Timmerhaus, *Plant Design and Economics for Chemical Engineers*, `TP 155.5.P4 1980`
- Sinnott, K., *Coulson and Richardson's Chemical Engineering*, volume 6, Chemical Engineering Design, `TP 155.5.C44 1993`
- Reid, R.C., J.M. Prausnitz and B.E. Poling, {em The Properties of Gases and Liquids}, 4th Ed., McGraw Hill (1987), `TP 242.R4 1987`
- *Kirk-Othmar Encyclopedia of Chemical Technology*, 4th Ed., `TP9.E685 1991`

- Encyclopedia of Chemical Processing and Design, J.J. McKetta, ed., `TP9.E66 V.69`
- Ullmann's Encyclopedia of Industrial Chemistry, `TP9.U57 1985`

Updated : The following results should be tabulated in your report:

Inlet temperature [K]	
Outlet temperature [K]	
Inlet pressure [Pa]	
Outlet pressure [Pa]	
Maximum tube-side temperature [K]	
Location from inlet of maximum temperature [m]	
Methanol production rate $[\text{kg.s}^{-1}]$	
Reactor length [m]	
Total inlet concentration, C_{T0} at 330K	
Rate constant, k_1 at 330K	
Equilibrium constant $K_{C,1}$ at 330K	
Rate constant, k_2 at 330K	
Equilibrium constant $K_{C,2}$ at 330K	
Heat of reaction for reaction 1 at 330K	
Heat of reaction for reaction 2 at 330K	

	Reactor in	Reactor out
Flow $[\text{mol.s}^{-1}]$		
Pressure [Pa]		
Temperature [K]		
CO (mole fraction) H_2 CO_2 CH_3OH H_2O		

New : A working set of MATLAB files must be emailed to the instructor with submission of your final report. These MATLAB files must generate the final profiles used to obtain the flows, pressure, temperature and mol fractions in the above tables. Non-working code, or code that does not lead to the values in the table will lead to a penalty in the grade.