CE 329 Fall 2015

Class 36 Worksheet[1]

Problem Purpose

This problem will allow you to practice setting up a 2-D tubular reactor model. It also highlights the importance of considering radial gradients when modeling exothermic reactions that are cooled through the tube wall.

Problem Statement

The partial oxidation of o-xylene to phthalic anhydride, reaction (1), is an exothermic reaction (ΔH = -307 kcal mol^{-1}). A heterogeneous catalyst for this reaction might consist of 3 mm particles with a bulk density of 1.3 g cm^{-3}, however this catalyst is sometimes mixed with an inert solid leading to an effective density of 0.87 g cm^{-3}. In either case, the catalyst is not perfectly selective, so that some of the o-xylene and some of the phthalic anhydride undergo total combustion to produce carbon oxides, reactions (2) and (3); the heat reaction (2) is -1090 kcal mol^{-1}. (The heat of reaction (3) equals the difference between the heats of reactions (1) and (2).) Letting A represent o-xylene, B represent phthalic anhydride and O represent oxygen, the rates for reactions (1) through (3) may be modeled using equations (4) through (6).

$$C_8H_{10} + 3\ O_2 \rightarrow C_8H_4O_3 + 3\ H_2O \tag{1}$$

$$C_8H_{10} \xrightarrow{O_2} CO_x \tag{2}$$

$$C_8H_4O_3 \xrightarrow{O_2} CO_x \tag{3}$$

$$r_1 = \left(4.122\times10^{11}\ \text{mol kg}^{-1}\ \text{h}^{-1}\right)\exp\left(\frac{-27\ \text{kcal mol}^{-1}}{RT}\right)P_AP_O \tag{4}$$

$$r_2 = \left(1.15\times10^{12}\ \text{mol kg}^{-1}\ \text{h}^{-1}\right)\exp\left(\frac{-31\ \text{kcal mol}^{-1}}{RT}\right)P_BP_O \tag{5}$$

$$r_3 = \left(1.73\times10^{11}\ \text{mol kg}^{-1}\ \text{h}^{-1}\right)\exp\left(\frac{-28.6\ \text{kcal mol}^{-1}}{RT}\right)P_AP_O \tag{6}$$

Consider a tubular reactor with an inside diameter of 1 inch and a length of 3 m that is cooled by perfectly mixed molten salts circulating outside the tube at a temperature equal to the feed temperature, 370 ºC. The mass velocity of the feed is 4684 kg m^{-2} h^{-1}; it consists of 0.93 mol% o-xylene in air which leads to a feed molecular weight of 29.48, a feed mole fraction of O_2 of 0.208 and a mass specific heat capacity of 0.25 kcal kg^{-1} K^{-1}, which may be assumed to be constant. Set up 2-D mole balances for o-xylene, phthalic anhydride and carbon oxides and a 2-D heat balance for this reactor assuming the superficial velocity to be constant, the wall heat transfer coefficient to equal 134 kcal m^{-2} h^{-1} K^{-1}, the

[1] This activity is based upon a case study from H. Rase, "Chemical Reactor Design for Process Plants," Vol. II. Wiley, New York, 1977.

effective radial conductivity to equal 0.67 kcal m^{-1} h^{-1} K^{-1} and the radial Peclet number for mass transfer (based on the superficial velocity and the catalyst particle diameter) to be constant and equal to 10. The first 75 cm of the tube is packed with the diluted catalyst, while the remainder contains the undiluted catalyst.

Rase states that solution of the 2-D model equations reveals maximum temperatures of 400 ºC (about two-thirds of the way into the part of the bed containing the diluted catalyst) and 410 ºC (about 25 cm after entering the part of the bed containing undiluted catalyst). Model this reactor as an ideal PFR with an overall heat transfer coefficient of 82.7 kcal m^{-2} h^{-1} K^{-1} (which is equivalent to the wall heat transfer coefficient and effective radial conductivity of the 2-D model) and compare the temperature maxima predicted by the PFR model to those reported for the 2-D model.

Worksheet

1. Read through the problem statement. Each time you encounter a quantity, write it down and equate it to the appropriate variable. When you have completed doing so, if there are any additional constant quantities that you know will be needed and that can be calculated from the values you found, write the equations needed for doing so.

2. Use the 2-D tubular reactor design equations found in Unit 34 or on the AFCoKaRE Exam Handout to generate an energy balance and mole balances on o-xylene, phthalic anhydride and carbon oxides. (Assume the stoichiometric coefficient of O2 to equal -8.5 in reaction (2) and -5.5 in reaction (3).)

3. Write the boundary conditions needed to solve the 2-D tubular reactor design equations and show how to calculate any new quantities they contain.

4. Using the PFR design equations from Unit 17 or the AFCoKaRE Exam Handout, generate the design equations needed to model this reactor as a PFR. Identify the specific set of equations that needs to be solved and within those equations identify the independent and dependent variables, if appropriate, and the unknown quantities to be found by solving the equations.

5. Assuming that the PFR design equations will be solved numerically, specify the information that must be provided and show how to calculate any unknown values.

6. Identify what variables will become known upon solving the design equations and show how those variables can be used to answer the questions that were asked in the problem.