CE 329 Fall 2015
Class 26 Worksheet

The irreversible oxidative dehydrogenation of ethane to ethylene, reaction (1), has a heat of reaction of -25 kcal mol^{-1}. It is first order in ethane; the pre-exponential factor for the rate coefficient is equal to 1.4 x 10^8 min^{-1} and the activation energy is 30 kcal mol^{-1}. The feed consists of 5% ethane in air at 350 °C and 2 atm; the heat capacity of the gas can be approximated to equal 3.5R and the pressure drop is negligible. The reactor has a diameter of 25 mm and is 2 m long Calculate the conversion and outlet temperature for a PFR operating at space times of 1, 10 and 50 min (a) assuming constant density and (b) accounting for the change in density.

$$C_2H_6 + ½\ O_2 \rightarrow C_2H_4 + H_2O \qquad (1)$$

Read through the problem statement and determine the type of reactor being used, whether it operates transiently or at steady state, whether it is heated/cooled, isothermal or adiabatic and (if the reactor is a PFR) whether there is a significant pressure drop

Read through the problem statement a second time and assign each quantity given in the problem statement to the appropriate variable symbol, if all of the given quantities are intensive, select a value for one extensive variable as the basis for your calculations and determine what quantities the problem asks for and assign appropriate variable symbols to them

Write a mole balance equation for each reactant and product, expanding all summations and continuous products and eliminating all zero-valued and negligible terms

Write an energy balance design equation, expanding all summations and continuous products and eliminating all zero-valued and negligible terms

If information about the heat transfer fluid, beyond its temperature, is provided or requested, write an energy balance on the heat transfer fluid

If the reactor is a PFR and there is a significant pressure drop, write a momentum balance, expanding all summations and continuous products and eliminating all zero-valued and negligible terms

Identify the type of the design equations as algebraic, ordinary differential or partial differential equations

if they are algebraic, identify a set of unknowns, equal in number to the number of equations

if they are differential, identify the independent and dependent variables, and if the number of dependent variables is greater than the number of equations, choose one dependent variable and express it and its derivatives in terms of the remaining dependent variables

Determine what you will need to provide in order to solve the design equations numerically and formulate the equations you need in order to do so

Write the necessary code and solve the design equations numerically

After the design equations have been solved numerically, use the results to calculate any other quantities or make any plots that the problem asked for