

CHE 4063 Project 2

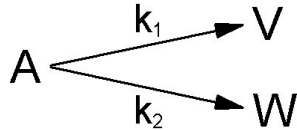
INSTRUCTIONS FOR PREPARING THE PROJECT

All pages should be 8 ½" x 11". Make xerox copies of all pages over 8 ½" x 11" including computer programs if necessary. Do not include any foldout pages.

1. Staple the project once in the upper left-hand corner. Do not use folders of any type.
2. Cooperation among students is forbidden.
3. Follow this format:
 - a. Cover page
 - b. Statement of the problem and data you were given.
 - c. Theoretical development including equations you developed and calculations you set up.
 - d. Results
 - i. Explanation and final numbers
 - ii. Graphical plots
 - e. Appendix – Computer program and raw data output.
4. Neatness and organization counts 10% of the project!

Computational tools used to solve this project are the students' choice. You may use a programming language such as C++, Visual Basic, or Fortran, or HYSYS.

The parallel reactions:



take place in a PFR. The gas phase reaction kinetics are known to be:

$$\begin{array}{ll}
 r_V = k_1 C_A^2 & \text{(Second order)} \\
 r_W = k_2 C_A & \text{(First order)}
 \end{array}$$

The following data are available:

$$\begin{array}{ll}
 A_V = 1.667 \times 10^4 \text{ lt/mole-sec} & A_W = 1.667 \times 10^5 \text{ sec}^{-1} \\
 E_V = 83,684 \text{ J/mole} & E_W = 125,526 \text{ J/mole} \\
 C_{P,V} = 29.29 \text{ J/mole-K} & C_{P,W} = 33.47 \text{ J/mole-K} \\
 \Delta H_V = -20,921 \text{ J/mole} & \Delta H_W = -62,763 \text{ J/mole}
 \end{array}$$

The reactor operates at 6 bar total pressure which may be assumed to be constant. The feed to the reactor is 100 moles/min of A and 500 moles/min of an inert material I. The heat capacities of A and I are 25.11 and 37.66 J/mole-K, respectively. All physical properties may be assumed independent of T and ideal gases may be assumed.

Provide plots of the following:

1. Y_V versus f_A for an isothermal reactor (of variable size) which operates at 700 K.
2. F_A , F_V , and F_W (all on the same graph) versus f_A for an isothermal reactor (of variable size) which operates at 700 K.
3. $Y_{V,EXIT}$ versus T_{IN} for an adiabatic reactor which has a space time $\tau = 3000$ seconds where T_{IN} varies from 650 - 750 K.
4. F_A , F_V , and F_W (all on the same graph) at the reactor exit versus T_{IN} for an adiabatic reactor which has a space time $\tau = 3000$ seconds where T_{IN} varies from 650 - 750 K. Find the inlet temperature which maximizes F_V at the reactor exit.