(1) The homogeneous gas decomposition of phosphine, $4 \text{ PH}_3(g) \rightarrow P_4(g) + 6$ $H_2(g)$, proceeds at 649°C with a rate constant of 10 hr^{-1} . What size plug flow reactor operating at 649°C and 460 kPa can produce 80% conversion of a pure feed consisting of 40 mol/h of pure phosphine? (20%)

Hint: R=8.31 Pa-m³/mol-K,
$$\int_{0}^{x} \frac{1+\epsilon x}{1-x} dx = (1+\epsilon) \ln \frac{1}{1-x} - \epsilon x$$

- (2) Please describe the condition of this rate law $(-r_A=kC_A^n)$ for that a CSTR give a smaller volume than a PFR for the same conversion. Of course, the operation parameters are the same for the CSTR and PFR, such as C_{A0} , temperature, volumetric flow rate...etc. (5%)
- (3) Make your sketches to get maximum selectivity of product D. Please describe the proper operation conditions, such as Temp, concentration. (5%)

A+B
$$\rightarrow$$
D -r_{1A}=10exp(-1000/T)C_A^{1.5}C_B^{0.5}
A+B \rightarrow U -r_{2A}=10⁹exp(-10000/T)C_AC_B

(4) Derive the rate law of substrate (r_s) for the following enzymatic reaction. (10%)

$$E + S \xrightarrow{k_1} E \cdot S$$

$$E \cdot S \xrightarrow{k_2} E + S$$

$$E \cdot S + W \xrightarrow{k_3} P + E$$

(5) The following liquid-phase reaction is carried out in an adiabatic CSTR without shaft work. Please calculate the reactor volume necessary to achieve 99% conversion. The formula obtained from energy balance of reactor temperature and conversion is: $T = T_0 + 43.4X$.

Additional information:

Feed = 150 kmol/h at 330K,
$$C_{A0}$$
=9.3M, C_{B0} =0,

E=65700 J/mol, k(360K) = 31.1 h⁻¹, K_c(333K)=3.03

 Δ H_{Rxn}(298K) = -6900 J/mol-A, R=8.31 J/mol-K

Hint: Van't - Hoff Relationship $\frac{d \ln K_c}{dT} = \frac{\Delta H_{Rxn}(T)}{RT^2}$ (10%)

(6) Species A is diffusing at steady state from the bulk fluid through a stagnant film of B of thickness δ to the external surface of a single catalyst pellet. The concentration of A at the external boundary is C_{Ab} . The surface reaction is so fast that it is not the rate-limiting step. Derive an expression for the mass flux

of A (W_{Ar}) to the catalyst surface at steady. What is the overall rate of reaction ($-r_{AS}$ ")? What happen to the overall rate of reaction when the catalyst pellet diameter (d_p) is reduced by one order of magnitude? (25%)

(7) The proposed reaction mechanism for the catalytic gas-solid reaction $A_{(g)}$ ---> $R_{(g)} + T_{(g)}$ is as follows:

$$A + S === A \cdot S \qquad (k_1, k_{-1})$$

$$A \cdot S + S === R \cdot S + T \cdot S \qquad (k_2, k_{-2})$$

$$R \cdot S === R_{(g)} + S \qquad (k_3, k_{-3})$$

$$T \cdot S === T_{(g)} + S \qquad (k_4, k_{-4})$$

where S is an active site and $A \cdot S$, $R \cdot S$ and $T \cdot S$ represent the species A, R and T, respectively, in the adsorbed state. The parameters k_i and k_{-i} (i = 1-4) in the parentheses represent the corresponding forward and reverse reaction rate constants, respectively. Immediately after the adsorption state, the adsorbed species is readily converted into products. This is followed by the rapid desorption of products. Derive the reaction rate law. For the isothermal irreversible reaction carried out in a packed bed reactor operated at very high temperature, propose methods that can increase the reaction rate. (25%)