CBE 450 Chemical Reactor Fundamentals
Midterm Exam 1
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Department of Chemical and Biomolecular Engineering
University of Tennessee, Knoxville

1. Write the five steps of Fogler's algorithm for solving reactor problems.

Solution:

1. Mole Balance
2. Stoichiometry
3. Rate Law
4. Combine
5. Evaluate

2. Consider an elementary elementary dimerization reaction of A to B (2A → B) in a batch reactor. Perform the five steps of Fogler's algorithm. Label each step. Introduce variables as necessary.

Solution:

1. Mole Balance

accumulation = in – out + generation

There is no in or out term in a batch reactor.

accumulation = generation

$$\frac{dC_A}{dt} = \nu_A r$$

2. Stoichiometry

This is an isomerization reaction of A to B.

2A → B

The stoichiometric coefficients are $\nu_A = -2$ and $\nu_B = 1$

3. Rate Law

This is an elementary reaction. Therefore the rate is of the form

$$r = kC_A^2$$

4. Combine

Substitute rate law and stoichiometry into the mole balance.

$$\frac{dC_A}{dt} = -2kC_A^{\ 2}$$

5. Evaluate

This ODE can be solved by hand.

$$\int_{C_{A,o}}^{C_A} \frac{dC_A}{C_A^{\ 2}} = -2\int_{t_o}^{t} kdt$$

$$-\left(\frac{1}{C_A} - \frac{1}{C_{A,o}}\right) = -2k(t - t_o)$$

Simplify

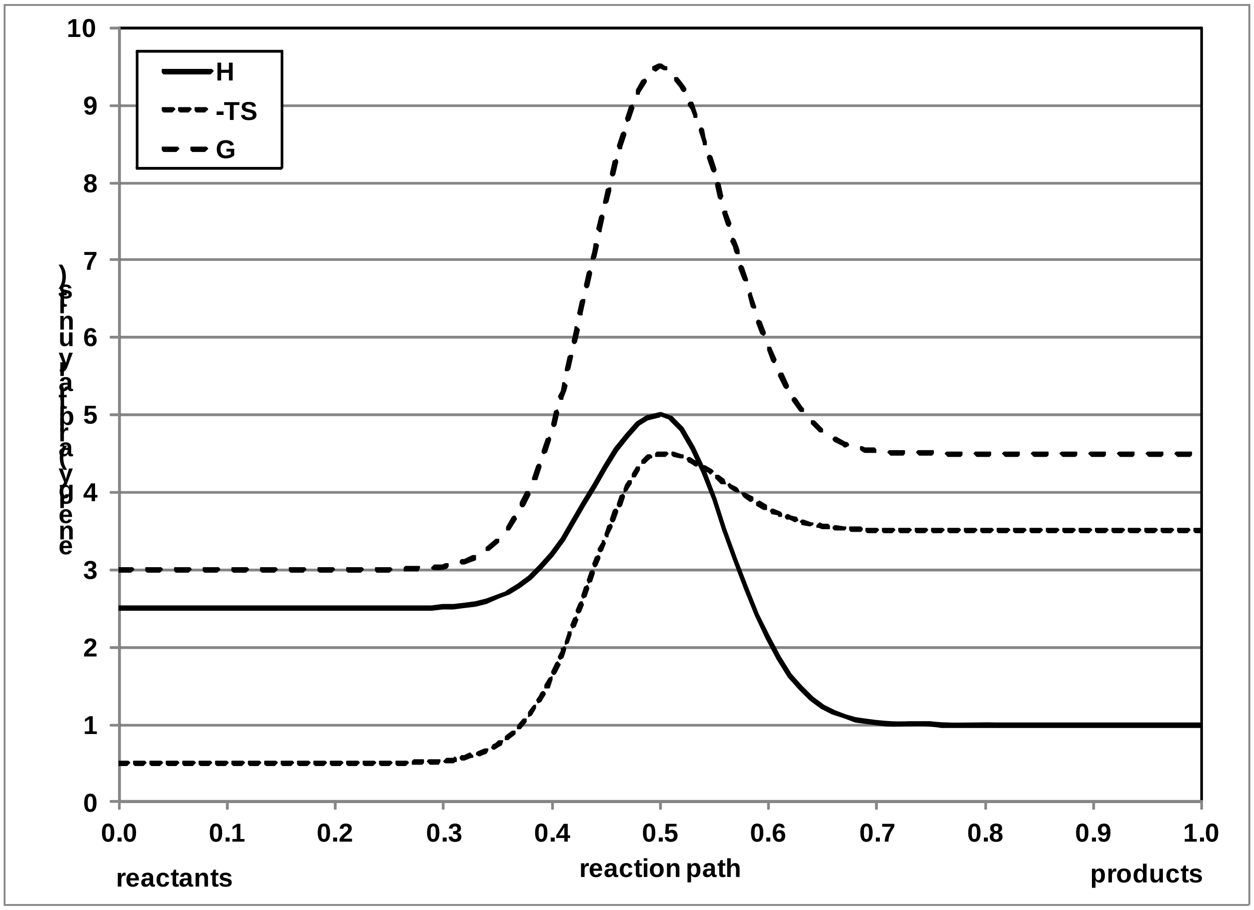
$$\frac{1}{C_A} = \frac{1}{C_{A,o}} + 2k(t - t_o)$$

$$C_A = \frac{1}{\frac{1}{C_{A,o}} + 2k(t - t_o)} = \frac{C_{A,o}}{1 + 2kC_{A,o}(t - t_o)}$$

3. For problem 2, derive an expression for conversion as a function of time in the reactor.

$$X_A = \frac{moles\,reacted}{moles\ provided} = \frac{C_{A,o} - C_A}{C_{A,o}} = 1 - \frac{C_A}{C_{A,o}} = 1 - \frac{\frac{C_{A,o}}{1 + 2kC_{A,o}(t - t_o)}}{C_{A,o}} = 1 - \frac{1}{1 + 2kC_{A,o}(t - t_o)}$$

4. Consider the thermodynamic properties at a given temperature shown in the following graph as a function of position along the reaction path for an isomerization reaction A → B.



(a) Is this reaction exothermic or endothermic? Why?
(b) At thermodynamic equilibrium, will there be greater moles of reactant or product in the mixture? Why?
(c) Will the equilibrium ratio of reactant to product increase or decrease as the temperature increases? Why?

Solution:

(a) Is this reaction exothermic or endothermic? Why?

This reaction is exothermic because the enthalpy of the product is less than the enthalpy of the reactants.

(b) At thermodynamic equilibrium, will there be greater moles of reactant or product in the mixture? Why?

At thermodynamic equilibrium, there will be greater moles of reactant than product because the free energy of the reactant is lower than the free energy of the reactant.

$$\frac{N_{reac\tan t}}{N_{product}} = K_{eq} = \exp\left(-\frac{G_{reac\tan t} - G_{product}}{RT}\right)$$

If $G_{reac\tan t} < G_{product}$, then the argument of the exponential is positive. The exponential of a positive number is greater than one, so the moles of reactant are greater than the moles of product.

(c) Will the equilibrium ratio of reactant to product increase or decrease as the temperature increases? Why?

$$\frac{N_{reac\tan t}}{N_{product}} = K_{eq} = \exp\left(-\frac{G_{reac\tan t} - G_{product}}{RT}\right)$$
$$= \exp\left(-\frac{H_{reac\tan t} - TS_{reac\tan t} - H_{product} + TS_{product}}{RT}\right)$$
$$= \exp\left(-\frac{-TS_{reac\tan t} + TS_{product}}{RT}\right)\exp\left(-\frac{H_{reac\tan t} - H_{product}}{RT}\right)$$
$$= \exp\left(-\frac{-S_{reac\tan t} + S_{product}}{R}\right)\exp\left(-\frac{H_{reac\tan t} - H_{product}}{RT}\right)$$

There is no temperature dependence in the entropic term. The temperature dependence lies in the enthalpic term. Therefore, if $H_{reac\tan t} > H_{product}$, then the argument of the enthalpic exponential is negative. As the temperature increases, the argument remains negative but the magnitude decreases. The exponential of a negative number is less than one. The smaller the magnitude of the negative number in the argument, the larger the exponential, which is the ratio of reactants to products. Therefore as temperature increases the fraction of reactant increases for this exothermic reaction.