**STOICHIOMETRY**

In order to calculate the concentration and the reaction rate law as a function of conversion for the following expression:



For the batch reactors, the reactor is opened at the start of the reaction and the reactants A, B and C are placed into the reactor. The number of moles of A remaining in the reactor after a conversion X has been achieved is:



In order to determine the number of moles of reactant B remaining at time t, for every mole of A that consumed, b/a moles of B must consumed; therefore, the number of moles of B that consumed is:



The number of moles of B remaining in the system at time t can be expressed as show below:



The expression in parentheses (c/a – b/a - 1) represent the increase in the total number of moles per mole of A reacted. This expression is shown with the symbol “δ”:



The total number of moles can now be calculated by using the given notation “δ” with the following equation:



In order to calculate the reaction rate as a function of conversion X, the concentrations of the reacting species need to be known as a function of conversion. The concentration of the reactants, A, B and C, are the number of moles of the reactants per unit volume as shown below:



The concentration expressions for B and C can be simplified by defining a new parameter as shown below:





For the constant-volume systems (V=Vo), the concentration expressions for A, B and C can be rearranged as shown below:



Table 1. Stoichiometry Table for the batch reaction system

The stoichiometric table for a continuous-flow system of the following reaction expression can prepared as shown below:



Table 2. Stoichiometry Table for a flow reaction system



For a flow system, the concentrations CA, CB and CC, at a given point can be determined from the molar flow rate FA, FB and FC and the volumetric flow rate v at that point. In order to calculate the concentration as a function of conversion X:



For liquid phase reactions, the volume change with reaction is negligible when no phase variation takes place.



**References:**

* H. Scott Fogler, “Elements of Chemical Reaction Engineering”, Prentice Hall Professional Technical Reference, Fourth Edition.