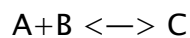# Mechanism and Elementary Reactions

In chapter 5 of my Reactor Design class, we learned about important differences between a reaction with apparent stoichiometry and the elementary reactions of the full reaction. Stoichiometry is the representation of quantities of reactants and products for the overall reaction. Elementary steps are the broken-down step by step reaction involving formation of intermediate steps. For more details, you can revisit my other post by clicking here. We also learned about the criteria of valid elementary steps for the overall stoichiometry. Additionally, the assumption that are typically made to simplify the rate expressions for complex reaction networks. Without further redue, let's get into the details!

The important difference between a reaction with an observed stoichiometry and an elementary reaction is that the stoichiometry of an elementary reaction defines the concentration dependence of the rate expression. The stoichiometric statements such as the one below are used to represent the changes that occur during a chemical reaction.

A+B <—> C

It might represent the change in the relative amounts of species that is observed when the reaction proceeds, or the actual molecular events that are presumed to occur as the reaction proceeds. However, an elementary reaction is characterized by a change from reactants to products that proceeds without the formation of identifiable intermediate species. Elementary reactions are usually unimolecular or bimolecular. On the other hand, any correspondence between the stoichiometric coefficients and the reaction order is purely coincidental. The elementary reactions are steps of the individual reactions to combine to give the overall observed stoichiometry.

A mechanism must pass the two simple tests to be considered a valid description of an overall stoichiometry. First of all, the elementary reactions must be able to be combined to form the overall stoichiometry. In other words, the mechanism for the individual unimolecular or bimolecular species must add up to the overall reaction. Secondly, the elementary reactions must be possible chemically for the reactants to form the products. In addition, the elementary reactions must also be kinetically significant to the appearance of products.

The two major assumptions that are made to simplify the rate expressions for complex reaction networks are listed as follows:

- The Reaction Equilibrium Assumption
  The full mechanism is reduced on the basis of fast and slow reactions. This is because some reactions equilibrate faster than the others. The slower reactions govern the rate at which the amounts of reactants and products change, also known as the rate-limiting step. The rate of the slow reaction determines the rate at which the concentrations change.
- The Quasi-Steady-State Assumption (QSSA)
  The full mechanism is reduced on the basis of rapidly equilibrating species. This is because in some cases the intermediates are transitory, highly reactive species that are chemically identifiable but unlikely to exist outside the reaction mixture. The way QSSA is done is to set the production rate of a reaction intermediate equal to zero.

Source: http://lehighcheme.wordpress.com/2014/04/21/mechanism-and-elementary-reactions/