Chemical reactor calculations are based on the elementary conservation laws of matter and energy. Information is required on flow phenomenon, rates at which the reactions precede heats of transformation, and description of chemical equilibrium.

Quantitative aspects of chemical Reactions:
Reactions may occur as soon as the reaction mixture is achieved to appropriate conditions of temperature and pressure with reactants well mixed in a molecular scale. Some of them require the use of catalyst which takes part on elementary steps. The catalyst may be under the same state as the reactants (homogeneous catalysts) or in a different state, usually the solid state (heterogeneous catalysts).

Classification of gross reaction types and reaction rates:
From a gross kinetic point of view, chemical reactions are mainly considered under overall formulations which do not refer to elementary processes. There are two classes of reactions
- the single reactions
- the multiple reactions

The single reactions comprise:
1. Uni-directional reactions
2. Reversible reactions

\[ v_A^A + v_B^B \rightarrow v_P^P + v_Q^Q \]

\[ v_A^A + v_B^B \rightarrow v_P^P + v_Q^Q \]
3. Autocatalytic reactions

\[ v_A^A \rightarrow Vp^P \]

Where the presence of the product P is necessary to provide the conservation of the reactant A.

The multiple reactions consist a wide variety of possible kinds of reactions, among which three basic types can be as follows:

- Parallel reactions

\[ v_{A_1}^A \rightarrow Vp_1^P \]
\[ v_{A_2}^A \rightarrow Vp_2^P \]
\[ A \rightarrow P \]
\[ \downarrow \]
\[ Q \]

Consecutive reactions

\[ V_{A_1}^A \rightarrow Vp_1^P \]
\[ V_{A_2}^A \rightarrow Vp_2Q \]
\[ A \rightarrow P \rightarrow Q \]

Complex reactions:

\[ V_{A_1}^A \rightarrow Vp_1^P \]
\[ V_{A_2}^A \rightarrow Vp_2Q \]
\[ V_{A_3}^A \rightarrow Vp_3X \]
\[ V_{A_4}^A \rightarrow Vp_4Y \]
\[ A \rightarrow P \rightarrow Q \]

The reaction formulation can be written under the form of a reaction balance. Thus for the reaction I this form gives:

\[ \sum_{j} v_{ij} A_{j} = 0 \]

Where \( A_{j} \) is the component \( j \) which corresponds to either a product or a reactant, and \( V_{ij} \) is the stoichiometry coefficient of the component \( A_{j} \) for the reaction \( i \). In this description \( v_{ij} \) is positive for a product and negative for a reactant.

Single reactions are described by a single reaction balance; multiple reactions are described by a system of reaction balances, the number of which is that of all the reactions involved.

In a single reaction I, the production rate of a given component is \( A_{j} \), defined by:

\[ r_{ij} = \frac{1}{V} \frac{\partial N_{j}}{\partial t} \]

Where, \( V \) = volume of reaction mixture
\( N_{j} \) = mole number of the component \( A_{j} \)

From the reaction stoichiometry, it can readily be established that \( r_{ij} / V \) is the same for all the components. This rate is called the kinetic rate of the reaction \( i \):

\[ r_{i} = \frac{r_{i}}{v_{ij}} \]

It can be noted that \( r_{i} \) is positive.

In the case of multiple reactions, the overall production rate of the component \( A_{j} \) is given by:

\[ R_{j} = \sum_{i} u_{ij} r_{ij} \]
The summation corresponds to all the reactions involved. Chemical reaction rates are expressed as functions of the concentrations or partial pressures. In the case where two reactants A and B are involved, the kinetic rate is most often expressed as:

\[ r = k C_A^m C_B^n \]  

...37.4

Where \( m \) and \( n \) are respectively the order of the reaction with respect to A, and the order with respect to B. The total order of the reaction is \( m+n \).

For reversible reactions, one has

\[ r = k_1 C_A^m C_B^n - k_2 C_P^p C_Q^q \]  

...37.5

And for autocatalytic reactions, this becomes

\[ r = k C_A^m C_P^p \]  

...37.6

For complex mechanism reactions formed by a combination of a number of elementary kinetic processes it is sometimes impossible to approximate the chemical reaction rate by one of the three equations above. The following types of rate equations can give better results:

\[ r = \frac{k C_A C_B}{1 + K_1 C_A + K_2 C_B} \]  

...37.7

\[ r = \frac{k C_A C_B}{\left[1 + K_1 C_A + K_2 C_B\right]^2} \]  

...37.8

In the chemical reaction rate equations, effect of temperature is taken into account in the reaction rate constant K which is expressed by:

\[ k = k_0 \exp(-E/RT) \]  

...37.9

It can be noted that the chemical reaction rate has been referred to the unit volume of the reaction mixture. However, for heterogeneous systems it can be to base it on another property. The volume of the liquid or the solids contained in the reactor, the mass of the solids or their internal or external surface area between two phases, etc. conversions from one to the other are easily obtained.

Relative degree of conversion, selectivity and yield:
The relative degree of conversion of a reactant A is a measure of the extent of the reaction. It is defined as the function of the amount of the reactant, fed in prior to and during the reaction, which has been converted:

\[ \zeta_A = \frac{N_{A0} - N_A}{N_{A0}} \]  \[\ldots 37.10\]

When products other than those desired are formed from the reactants A and B, it is convenient to use the concept of selectivity and yield. The selectivity of a desired product with respect to a key reactant A is the ratio between the amount of P obtained and the amount of A converted. These amounts must take into account the stoichiometry of the reaction.

\[ s_A = \frac{N_P - N_{P0} v_A}{N_{A0} - N_A v_p} \]  \[\ldots 37.11\]

The yield of the product P with respect to the key component A is the ratio of the amount of P obtained to the amount of A fed in, corrected for the stoichiometry considerations:

\[ \eta_P = \frac{N_P - N_{P0} v_A}{N_{A0} v_p} \]  \[\ldots 37.12\]

By combining equations (37.10 and 37.12) we obtain

\[ \eta_P = s_A \zeta_A \]  \[\ldots 37.13\]

**Classification of reactors:**

- Homogeneous systems
- Heterogeneous systems
  - Homogeneous systems are autoclave reactors, tubular reactors.
  - Fixed bed, fluidized bed, mixing bed etc.

**Homogeneous systems:**

- batch reactor (BR) – under isothermal conditions
- semibatch reactors – under isothermal conditions
- CSTR → steady state
  ↓
  -under isothermal conditions
  Unsteady state
- plug flow → steady state
  ↓
  -under isothermal conditions
Unsteady state