**Theory:**

The schematic of a reactor is shown in the figure below:

NC (Inlet flow) NC (Outlet flow)

Reactor with specific T, P

The mass balance for the reactor is written as follows:

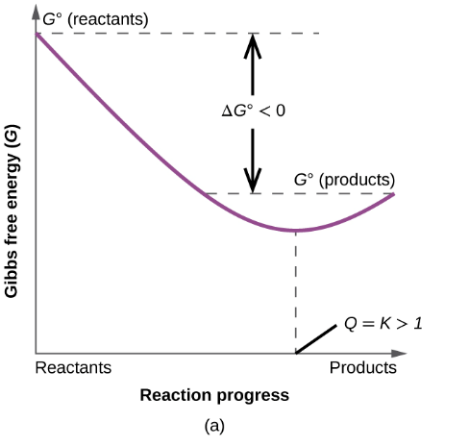
Last Session, we define as extent of reaction, and it is written as follows:

Thie main task is to find using equilibrium data in the outlet flow of the reactor.

The first thing we must know is *how many reactions we need to fully define the system*. To find the number of reactions, we can use this formula:

And [A] term is the rank of A matrix (matrix of species). It shows how many nonlinear independent elements we have.

The next issue is how to find . With Gibbs-free energy versus Reaction Coordinate plot, we can determine with calculate global minimum of this plot, which mathematically is described as follows:



Next step is to calculate partial derivative of this equation:

The chemical Potential () cannot be calculated directly. Respect to Lewis’s equation we have:

The ratio “” described as activity coefficient (ai­)

Thus, the equation will be converted to:

Additionally, the equation above will be converted to:

In thermodynamics we have 3 cases in order to determine fugacity:

*In Ideal Mixture – Real Gas case, the value of fugacity is fixed.*

By knowing the fugacity of each component, we can determine the fugacity of mixture. This is very complicated from the numerical point of view.

1. **T effect @ constant P:**

Vant Hoff equation:

If , it indicates that we have an exothermic reaction. The increasing of T leads to decreasing .

Otherwise, we have an endothermic reaction. The decreasing of T leads to increasing .

1. **P effect @ constant T**

Suppose a reaction like this:

The equilibrium constant will be expressed as follows:

if c+d > a+b: With increasing pressure, the term will be decreased.

Elseif c+d < a+b: With increasing pressure, the term will be increased.

Else: With increasing pressure, the term will be constant.

The schematic of all system is shown in the figure below:

A diagram of a flowchart

Description automatically generated

The reactions are written as follows:

To find y2, we must write a mass balance:

To find y1, we must assign a basis of calculation, e.g. 100 mol/s.