Lecture #7. **Modeling of chemical reactions**

Key Equations and Laws in Reaction Modeling

Reaction **rate** equation often takes the form

$$r = k[A]^m[B]^n$$

where r is the reaction rate, k is the rate constant, and [A] and [B] are the equilibrium concentrations of reactants.

Arrhenius equation describes the **temperature** dependence of the reaction rate constant,

$$k = Ae^{-E_a/RT}$$

Equilibrium constant – K for a reaction:

$$aA+bB=cC+dD$$

$$K = \frac{[C]^c[D]^d}{[A]^a[B]^b}$$

Modeling the Haber-Bosch Process

The Haber-Bosch process synthesizes ammonia (NH_3) from nitrogen (N_2) and hydrogen (H_2), a key process in producing fertilizers.

Goal of Modeling: To predict ammonia production rate under varying conditions (e.g., high pressure, specific temperature ranges) and improve reactor efficiency.

Impact of Modeling: Using this model, the chemical industry can optimize energy usage, reduce costs, and enhance output.

Chemical Reaction: $N_2+3H_2 \leftrightarrow 2NH_3$

The rate of this reaction is influenced by temperature, pressure, and catalyst presence.

Modeling Components:

- *Rate Equation:* The rate law for the reaction considers the partial pressures of nitrogen and hydrogen.
- *Temperature Effects:* Using the Arrhenius equation, the model accounts for how different temperatures impact the rate.
- *Equilibrium Consideration:* The equilibrium constant changes with temperature, helping determine optimal conditions for maximizing ammonia yield.

Modeling the Haber-Bosch process helps illustrate the power of chemical reaction modeling in industrial applications, demonstrating how equations and reaction principles guide real-world decision-making and optimization.