

## Lecture #7. Modeling of chemical reactions

### Key Equations and Laws in Reaction Modeling

Reaction **rate** equation often takes the form

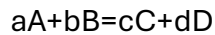
$$r = k[A]^m[B]^n$$

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:



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

### Modeling the Haber-Bosch Process

The Haber-Bosch process synthesizes ammonia ( $\text{NH}_3$ ) from nitrogen ( $\text{N}_2$ ) and hydrogen ( $\text{H}_2$ ), 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:**  $\text{N}_2 + 3\text{H}_2 \rightleftharpoons 2\text{NH}_3$

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.