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

Goal

This lecture introduces students to the principles and mathematical foundations of chemical reaction modeling. Students will learn how to formulate rate equations, apply the Arrhenius law and equilibrium relationships, and use modeling to analyze and optimize real chemical processes. The Haber–Bosch process for ammonia synthesis is used as a key example to illustrate how reaction kinetics, temperature effects, and equilibrium conditions are combined in industrial reaction modeling.

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.

Learning Outcomes

By the end of this lecture, students will be able to:
1. Explain the fundamental laws and equations governing chemical reactions, including the rate law, Arrhenius equation, and equilibrium constant (related to LO 4, ID 4.3).
2. Formulate rate expressions for single and multiple reactions using concentration or partial-pressure terms (related to LO 4, ID 4.3–4.4).
3. Apply the Arrhenius equation to model the effect of temperature on reaction rate constants (related to LO 4, ID 4.3–4.4).
4. Use equilibrium relationships to evaluate reaction yields under various temperature and pressure conditions (related to LO 4, ID 4.3–4.5).
5. Model and interpret an industrial example — the Haber–Bosch process — by integrating kinetic and equilibrium principles to predict and optimize ammonia production (related to LO 4, ID 4.5–4.6).

6. Discuss the role of reaction modeling in process design, catalyst development, and energy efficiency improvement (related to LO 4, ID 4.6–4.7).

Questions and Self-Study Assignments

1. Define the rate law and explain how it differs for first- and second-order reactions.

2. Using the Arrhenius equation, calculate how the rate constant changes when the temperature increases from 500 K to 600 K for a reaction with Ea = 100 kJ/mol.

3. Write the rate expression in terms of partial pressures.

4. Discuss how pressure influences the forward and reverse reactions.

5. Explain why increasing temperature both accelerates reaction kinetics and decreases ammonia yield in the Haber–Bosch process.

6. Plot qualitatively (no calculations needed) how equilibrium conversion of N_2 to NH_3 changes with temperature and pressure.

7. Describe how modeling assists in reactor design and catalyst selection for industrial ammonia synthesis.

8. Read a recent (within 3 years) article on kinetic modeling of catalytic reactions and summarize:

- main equations used;

- temperature dependence analyzed;

- practical implications for industrial optimization.

References

1. Finlayson B.A. Introduction to Chemical Engineering Computing. Second Edition. - John Wiley & Sons, 2012., DOI: 10.1002/9781118309599

2. Pryor R.W. Multiphysics Modeling Using COMSOL5 and MATLAB. - Mercury Learning and Information, 2015. – 700 p.