Lecture 11 Energy Analysis of Reactors: Thermal Effects and Heat Balance

Goal of the lecture: To study the thermal behavior of chemical reactors, analyze heat generation and removal during reactions, and develop heat balance equations to ensure stable reactor operation.

Brief lecture notes: This lecture focuses on understanding how energy transformations occur inside chemical reactors and how heat effects influence reaction rates, conversion, and safety. We will explore the sources of heat in chemical reactions, derive the energy balance equations for different reactor types, and analyze steady-state and dynamic temperature profiles. Special attention will be given to the interaction between kinetics and heat transfer, adiabatic and non-adiabatic conditions, and methods of thermal stabilization in industrial processes.

Main part

Every chemical reaction involves a change in energy — either releasing heat (*exothermic reactions*) or absorbing it (*endothermic reactions*). The thermal effect per mole of reaction can be expressed as the enthalpy of reaction:

$$\Delta H_r = \sum \nu_p H_p - \sum \nu_r H_r$$

where ν_p, ν_r are stoichiometric coefficients, and H_p, H_r are the molar enthalpies of products and reactants, respectively.

In reactor design, understanding these thermal effects is essential for predicting temperature rise, heat transfer needs, and operational stability.

Energy Balance Equation for Reactors

The general energy balance for a steady-state reactor can be expressed as:

$$\dot{Q} + \dot{W} + \sum \dot{n}_{in} h_{in} = \sum \dot{n}_{out} h_{out}$$

where:

- $\dot{Q}$ — rate of heat transfer,
- $\dot{W}$ — work done (often negligible in most reactors),
- $\dot{n}$ — molar flow rate,
- h — specific enthalpy.

For most chemical reactors (no shaft work), the simplified form becomes:

$$\rho C_p \frac{dT}{dt} = (-\Delta H_r) r + \frac{UA}{V}(T_j - T)$$

Here r is the reaction rate, U — heat transfer coefficient, A — surface area, V — reactor volume, and T_j — coolant (jacket) temperature.

This equation links reaction heat generation and heat removal, determining the thermal stability of the system.

Thermal Behavior in Different Reactor Types

Reactor Type	Thermal Feature	Energy Balance Characteristics
Batch Reactor	No flow; temperature changes with time	Unsteady-state balance involving dT/dt
CSTR (Continuous Stirred-Tank Reactor)	Well-mixed; uniform temperature	Steady-state energy balance; possible multiple steady states

Reactor Type	Thermal Feature	Energy Balance Characteristics
PFR (Plug Flow Reactor)	Temperature varies along reactor length	Differential balance with respect to position dT/dz

- Adiabatic reactors have no heat exchange with surroundings; temperature changes depend solely on reaction heat.
- Isothermal reactors maintain constant temperature via heat exchangers or cooling jackets.
- Non-isothermal reactors show strong coupling between reaction rate and temperature — often leading to runaway or oscillatory behavior if not properly controlled.

Heat Transfer and Control Methods

Efficient heat management is essential to maintain optimal reaction conditions and prevent thermal hazards.

Methods include:

- Cooling/heating jackets for CSTRs.
- Internal or external heat exchangers.
- Multi-stage reactors to distribute heat generation.
- Use of diluents or inert gases to moderate exothermicity.

Example: In an exothermic CSTR, the steady-state temperature is found from the intersection of the heat generation curve ($q_{gen} = -\Delta H_r r$) and heat removal curve ($q_{rem} = UA(T - T_j)$). Multiple intersections indicate possible multiple steady states, where one may be stable and another unstable.

Example: Adiabatic Temperature Rise

The temperature rise in an adiabatic reactor can be estimated from:

$$\Delta T_{ad} = \frac{(-\Delta H_r)X}{\sum_i \quad n_i C_{p,i}}$$

where $X$is the conversion, and the denominator represents the total heat capacity of the reacting mixture.

This relation helps estimate how much the temperature will increase if no cooling occurs — critical for reactor safety design.

Figure 1.

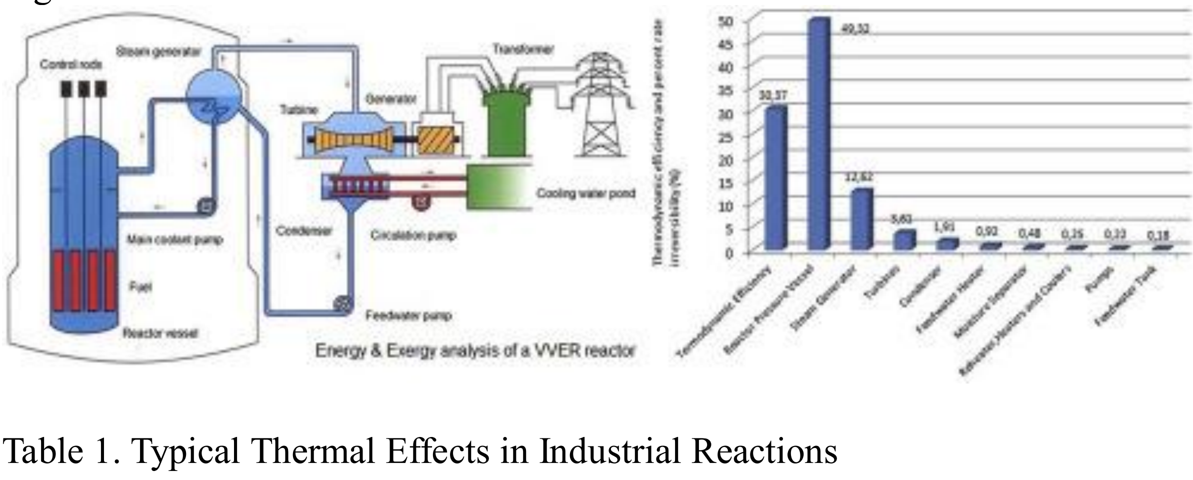

Table 1. Typical Thermal Effects in Industrial Reactions

Reaction	Type	ΔH (kJ/mol)	Thermal Control Strategy
Hydrogenation of ethylene	Exothermic	-137	Cooling jacket or external exchanger
Steam reforming of methane	Endothermic	+206	Furnace or radiant heating
Ammonia synthesis	Exothermic	-92	Multi-bed reactor with intercooling
Methanol synthesis	Exothermic	-91	Recycle with heat recovery
Dehydrogenation of ethylbenzene	Endothermic	+124	High-temperature heat input

Questions for Self-Control

1. What is the significance of the energy balance equation in reactor design?
2. How do adiabatic and isothermal reactors differ in their thermal behavior?
3. What conditions can lead to thermal runaway in exothermic reactions?
4. Explain how the heat generation and removal curves determine reactor stability.
5. How is adiabatic temperature rise calculated, and why is it important?

Literature

1. Fogler H. S. Elements of Chemical Reaction Engineering, 5th ed. – Prentice Hall, 2016.
2. Levenspiel O. Chemical Reaction Engineering, 3rd ed. – Wiley, 1999.
3. Smith J. M., Van Ness H. C., Abbott M. M. Introduction to Chemical Engineering Thermodynamics, 8th ed. – McGraw-Hill, 2017.
4. Baerns M., Hofmann H., Renken A. Chemical Reactor Analysis and Design Fundamentals. – Wiley-VCH, 2013.
5. Froment G. F., Bischoff K. B. Chemical Reactor Analysis and Design, 3rd ed. – Wiley, 2010.