**NOTES**

**Examples of Regression in Chemical Engineering:**

Regression is everywhere in **chemical engineering**, because we often need to **fit experimental data** to a model. Let me give you concrete **examples of regression applications** in chemical engineering:

**1. Kinetics & Reaction Engineering**

* **Rate constant determination**  
  Fit experimental concentration–time data to:

Regression gives the best-fit k.

* **Reaction order determination**  
  Regression on vs. t (first-order) or 1/CA vs. t (second-order).

**2. Thermodynamics**

* **Vapor–liquid equilibrium (VLE) data fitting**  
  Use regression to fit activity coefficient models (e.g., NRTL, Wilson, UNIQUAC) to experimental VLE data.
* **Equation of state (EOS) parameter fitting**  
  Fit van der Waals, Peng–Robinson, Soave–Redlich–Kwong parameters to PVT data.

**3. Transport Phenomena**

* **Diffusion coefficients**  
  Fit experimental concentration profiles to Fick’s law solutions to estimate D.
* **Heat transfer correlations**  
  Regression to obtain coefficients in Nusselt number correlations:

Nu=CRemPrn

**4. Process Design**

* **Pump/compressor performance curves**  
  Regression to fit polynomial/empirical curves:

H=a+bQ+cQ2

* **Distillation column design**  
  Regression of equilibrium data for McCabe–Thiele method.

**5. Materials & Nanotechnology**

* **Adsorption isotherms**  
  Regression of qe vs. Ce data to Langmuir or Freundlich models:
* **Catalyst characterization**  
  Regression of BET adsorption isotherm for surface area.

**6. Process Control**

* **System identification**: Regression used to fit experimental input–output data to transfer functions:

**Summary**:  
Regression in chemical engineering is commonly used in:

* **Reaction kinetics** (rate constants, reaction orders)
* **Thermodynamics** (EOS, activity coefficient models)
* **Transport** (diffusion, heat transfer correlations)
* **Design correlations** (pump, compressor, reactor data)
* **Adsorption/Material science** (isotherms, BET)
* **Control** (process dynamics, transfer functions)

**Examples of Interpolations in Chemical Engineering:**

Interpolation is widely used in chemical engineering whenever we need to **estimate unknown values between known experimental or tabulated data points**. Here are some **examples of interpolations in chemical engineering**:

1. **Thermodynamics & Properties**
   1. **Steam tables / Refrigerant tables**
   * Interpolating between tabulated values of **enthalpy, entropy, specific volume, internal energy** at a given temperature and pressure.
   * Example: Estimating enthalpy at 260 °C and 12 bar when only 250 °C and 270 °C data are available.
   1. **Heat capacity (Cp) data:** Cp values are often given at discrete temperatures. Interpolation is used to get Cp at an intermediate temperature for energy balance calculations.
   2. **Viscosity & thermal conductivity of fluids:** These are usually available at discrete T and P values. Engineers interpolate to get values at required operating conditions.
2. **Reaction Engineering**
   1. **Reaction rate constants (Arrhenius parameters):** Interpolating experimental rate constant data at intermediate temperatures if Arrhenius plot is not fitted yet.
   2. **Conversion vs. time data in batch reactors:** Interpolation is used when experimental points are available at specific times but conversion is needed at intermediate times.
3. **Mass Transfer & Separation Processes**
   1. **Diffusion coefficient data:** Values are often available at limited conditions. Interpolation helps in estimating at intermediate pressures/temperatures.
   2. **Distillation column design**
   * Relative volatility values or equilibrium compositions (x-y data) from VLE diagrams are interpolated.
   * Example: Bubble point or dew point calculations require interpolation in T-x or P-x-y data.
4. **Fluid Flow**
   1. **Friction factor (Moody chart / Colebrook equation):** When the Moody chart is used, interpolation is necessary between data points of Reynolds number and relative roughness.
   2. **Pump/compressor performance curves:** Head vs. flow rate or efficiency vs. flow data is often tabulated. Interpolation is used to predict performance at operating points not given in the manufacturer’s data.
5. **Process Data Analysis**
   1. **Experimental calibration curves**
   * Interpolating absorbance vs. concentration in spectroscopy (Beer–Lambert law).
   * Example: In chemical analysis, concentration is interpolated from standard calibration curves.
   1. **Process control & instrumentation:** Control valves: flow coefficient (Cv) data is interpolated for intermediate valve positions.

Interpolation is most commonly used in **property estimation (thermodynamics, transport), experimental data analysis, process design (distillation, heat exchangers, pumps), and kinetics**.

**Examples of Linear equations in Chemical Engineering:**

In chemical engineering, **linear equations** arise when system variables are related in a linear way. Often, they appear in **material balances, energy balances, transport equations, and process models**.

Here are some **examples of linear equations in chemical engineering**:

**1. Material Balance**

* **Steady-state mixing problem**  
  If two streams mix to form an outlet stream:

F1C1+F2C2=F3C3

where F = flow rate, C = concentration.  
→ This is a linear equation in terms of flow rates and concentrations.

**2. Energy Balance**

* **Heat exchanger (simple case)**

→ Linear relation between heat duty Q and temperature difference.

**3. Fluid Flow**

* **Darcy’s law for laminar flow through a packed bed**

where ΔP= pressure drop, v = superficial velocity, K = constant.  
→ Linear equation.

* **Hagen–Poiseuille law (in terms of flow rate vs. pressure drop)**  
  For laminar flow in a pipe:

→ Linear relation between flow rate Q and pressure drop ΔP.

**4. Reaction Engineering**

* **First-order rate law expressed as linearized equation**

→ Straight-line form: y=mx+c.

* **Batch reactor mole balance (constant volume)**

(after integration, gives the linearized form above).

**5. Process Control**

* **Linearized dynamic equations**  
  Small deviations around steady state often reduce nonlinear models to linear forms:

where y = output, u = input.

**6. Numerical Methods in Chemical Engineering**

* **Systems of linear equations** arise in:
  + Solving **simultaneous material balances** for multi-unit processes.
  + **Heat conduction in a rod (finite difference method):**

(Linear algebraic equation for interior nodes).

**Summary**:  
Linear equations show up in chemical engineering in **mass balances, energy balances, transport laws (Darcy’s, Hagen–Poiseuille, Fourier’s simplified), reaction rate plots, and discretized PDEs**.

In chemical engineering, **simultaneous linear equations with 3 unknowns** often come from **material balances, energy balances, or process models**.

**Example 1: Material Balance in a Mixing Process**

Three streams mix to form a product stream. Let x,y,z be the flow rates of the three streams.

Equations:

**Example 2: Heat Balance in a 3-Unit Network**

Suppose three heat exchangers supply unknown heats Q1,Q2,Q3.

Equations:

**Example 3: Reaction Stoichiometry (Simultaneous Material Balances)**

Consider a reactor with three unknown outlet molar flow rates a,b,c.

Equations:

**Examples of Non-Linear Equations in Chemical Engineering:**

In chemical engineering, **non-linear equations** appear very frequently, because many real processes involve **exponential, logarithmic, power-law, and product terms of variables**. These equations usually cannot be solved directly by linear algebra, and need **iteration / numerical methods** (Newton–Raphson, successive substitution, etc.).

Here are some **examples of non-linear equations in chemical engineering**:

**1. Reaction Engineering**

* **Arrhenius equation (temperature dependence of rate constant):**

→ Exponential, hence non-linear.

* **Rate laws with higher order:**

→ Power-law form, non-linear in CA.

* **CSTR design equation (non-linear for first-order kinetics):**

(because CA appears in denominator).

**2. Thermodynamics**

* **Equation of State (EOS):**
  + Van der Waals equation:

→ Non-linear in Vm.

* + Redlich–Kwong, Peng–Robinson EOS also give **cubic non-linear equations** in molar volume or compressibility factor Z.
* **Activity coefficient models:**  
  Example: Wilson, NRTL, UNIQUAC models use **exponentials and logarithms** of mole fractions.

**3. Mass Transfer & Separation**

* **Vapor–liquid equilibrium (Raoult’s law + Antoine equation):**

→ Non-linear in temperature T.

* **Distillation stage calculations (McCabe–Thiele rigorous):**  
  → Non-linear in composition.

**4. Fluid Flow**

* **Colebrook equation for friction factor:**

→ Highly non-linear, solved iteratively.

* **Bernoulli’s equation with friction losses:**

(non-linear because ff depends on Reynolds number, which itself depends on velocity v).

**5. Heat Transfer**

* **Radiation heat transfer:**

→ Non-linear due to the T4 term.

* **Non-linear heat conduction:**  
  If thermal conductivity depends on temperature k(T), the governing PDE becomes non-linear.

**6. Process Control**

* **Non-linear dynamic models:**  
  Example: CSTR energy balance with heat removal:

→ Non-linear because .

**Summary:**  
Non-linear equations in chemical engineering appear in **EOS (thermodynamics), reaction rate expressions, mass transfer (VLE), fluid flow (friction factor), radiation heat transfer, and dynamic reactor balances**.

**Examples of Ordinary Differential Equations in Chemical Engineering:**

Ordinary Differential Equations (ODEs) show up everywhere in chemical engineering whenever we describe **rates of change of concentration, temperature, pressure, or other variables with respect to time or one dimension**.

Here are some **examples of ODEs in chemical engineering**:

## **1.** **Reaction Engineering**

* **Batch reactor mole balance (first-order reaction):**

→ ODE in time, concentration decreases exponentially.

* **Second-order reaction in batch reactor:**
* **Autocatalytic reaction:**

## **2.** **Heat Transfer**

* **Newton’s law of cooling (lumped system):**

→ First-order ODE describing cooling of a body.

* **Heating/cooling of a CSTR jacket:**

## **3. Mass Transfer**

* **Unsteady diffusion in a thin film (1D Fick’s law lumped form):**

(after lumping in one dimension → ODE form).

* **Gas absorption in a stirred tank:**

→ ODE describing change in solute concentration with time.

## **4. Fluid Mechanics**

* **Unsteady tank draining (Torricelli’s law):**

where h = liquid height, a = orifice area, A = tank area.

* **Momentum balance in unsteady flow:**

mdvdt=F−f(v)

## **5. Process Control / Dynamics**

* **First-order linear system (e.g., level in a tank):**

→ ODE governing response to input u(t).

* **Second-order system (e.g., spring-mass-damper analogy in chemical process):**

**Summary:**  
Ordinary Differential Equations in chemical engineering appear in:

* **Reaction engineering** (batch reactor concentration change),
* **Heat transfer** (cooling/heating of objects, CSTR energy balances),
* **Mass transfer** (gas absorption, unsteady diffusion),
* **Fluid mechanics** (unsteady flow, draining tanks),
* **Process control** (dynamic system response).

Do you want me to also include **PDE vs ODE examples** (like heat conduction PDE vs lumped ODE cooling) to make the distinction clearer for your students?

**Examples of Partial Differential Equations in Chemical Engineering:**

Partial Differential Equations (PDEs) are very common in **transport phenomena** (momentum, heat, and mass transfer) and **reactor design**, because these processes depend on **both time and space variables**.

Here are some **examples of PDEs in chemical engineering**:

## **1. Heat Transfer**

* **Unsteady-state (transient) heat conduction equation:**

where α=kρCp (thermal diffusivity).  
→ PDE in **time** and **space coordinates**.

* **Heat conduction with internal heat generation:**

## **2.** **Mass Transfer**

* **Fick’s second law of diffusion (transient diffusion):**
* **Convection–diffusion equation (important in reactors, separation):**

→ Appears in packed-bed reactors, absorption columns.

## **3.** **Fluid Mechanics**

* **Continuity equation (for compressible fluids):**
* **Navier–Stokes equation (momentum balance):**

ρ∂v∂t+ρ(v⋅∇)v=−∇P+μ∇2v

→ Non-linear PDE in velocity and pressure.

## **4. Reaction Engineering**

* **Diffusion–reaction in a catalyst pellet:**

→ PDE combining diffusion and reaction inside porous catalysts.

* **Plug flow reactor with axial dispersion (PDE model):**

## **5.** **Process Control & Transport**

* **Distributed parameter systems (PDE models in control):**  
  Example: Temperature distribution in a long pipe:

**Summary:**  
Partial Differential Equations in chemical engineering are found in:

* **Heat transfer** → transient conduction, conduction with generation.
* **Mass transfer** → transient diffusion, convection–diffusion.
* **Momentum transfer** → Navier–Stokes, continuity.
* **Reaction engineering** → diffusion–reaction in catalysts, axial dispersion model of PFR.
* **Process systems** → distributed parameter models (temperature/concentration profiles in reactors & pipes).

In thermodynamics, PDEs arise when **state properties (T, P, V, U, S, H, etc.) depend on more than one independent variable**. Many of these are **fundamental thermodynamic relations** or **transport-thermodynamics couplings**.

**Examples of PDEs in Thermodynamics**

**1. Fundamental Thermodynamic Relations**

* From the first law:

dU=TdS−PdV

Since U is a function of entropy S and volume V:

∂U/∂S∣V=T, ∂U/∂V∣S=−P

→ These are **PDE relationships** between thermodynamic properties.

**2. Maxwell Relations (from Gibbs free energy)**

Derived from exact differentials of thermodynamic potentials, e.g.:

∂T/∂V∣S=−∂P/∂S∣V

∂T/∂P∣S=∂V/∂S∣P

→ Each is a PDE linking state functions.

**3. Clapeyron Equation (Phase Equilibrium)**

dP/dT=ΔHtrans/T ΔVtrans

This comes from applying **PDE relationships** between entropy, enthalpy, and volume across a phase boundary.

**4. Heat Conduction (Thermodynamic Transport)**

* Governing PDE (Fourier’s law + first law):

∂T/∂t=α∇2T

where α=k/(ρCp).  
→ A PDE in **time** and **space**, used for transient heat transfer in thermodynamics.

**5. Entropy Balance in a Control Volume**

From second law:

∂(ρs)∂t+∇⋅(ρsv)=σs

where σs≥0 is the entropy generation rate.  
→ PDE describing **entropy distribution** in space and time.

**6. Equation of State in PDE Form**

For compressible fluids:

∂P/∂T∣V=∂S/∂V∣T

This comes from thermodynamic consistency and links EOS with entropy.

**Summary**

PDEs in thermodynamics appear in:

* **Fundamental relations** (internal energy, enthalpy, Gibbs/Helmholtz potentials).
* **Maxwell relations** (cross-derivative PDEs).
* **Clapeyron/Clausius–Clapeyron equations** (phase equilibria).
* **Heat conduction PDE** (linking thermodynamics and transport).
* **Entropy balance PDEs** (2nd law applications).
* **Equations of state in differential form** (thermodynamic consistency).

**Examples of Definite Integrals in Chemical Engineering:**

**Definite integrals** are very common in chemical engineering because we often deal with **cumulative quantities** (heat, work, mass, concentration) over an interval.

## **1. Material Balance & Reaction Engineering**

* **Batch reactor conversion (first order reaction):**

X=∫0tk e−kt dt

Integrating gives the conversion as a function of time.

* **Residence Time Distribution (RTD):**

∫0∞E(t) dt=1

(Normalization condition for RTD function).

## **2.** **Thermodynamics**

* **Work done during expansion/compression of gases:**

W=∫V1V2P dV

e.g. Isothermal expansion:

W=nRT∫V1V2dVV=nRTln⁡V2V1

* **Change in enthalpy/entropy:**

ΔH=∫T1T2Cp(T) dT

ΔS=∫T1T2Cp(T)T dT

## **3.** **Heat Transfer**

* **Heat flux through a wall with varying conductivity:**

q=∫0Lk(T) dTdx dx

* **LMTD derivation (Log Mean Temperature Difference):**  
  Total heat transfer in an exchanger:

Q=UA∫0LΔT(x) dx

## **4.** **Mass Transfer**

* **Total diffusion flux across a film:**

NA=−DAB∫CA1CA2dCAdx dx

* **Absorption rate in a packed column:**

R=∫0HkLa (CA∗−CA(z)) dz

## **5.** **Fluid Mechanics**

* **Velocity profile integration (pipe flow):**  
  For laminar flow:

Q=∫0Ru(r) 2πr dr

where u(r)=ΔP4μL(R2−r2).

* **Shear stress distribution:**

## **6.** **Process Design & Data Analysis**

* **Cumulative energy consumption:**
* **Numerical integration of experimental data (trapezoidal, Simpson’s rule)**  
  Used in calorimetry, titration curves, adsorption isotherms.

✅ **Summary:**  
Definite integrals in chemical engineering appear in:

* **Reaction engineering** → conversion, RTD.
* **Thermodynamics** → work, enthalpy, entropy.
* **Heat transfer** → wall conduction, LMTD.
* **Mass transfer** → diffusion flux, absorption.
* **Fluid mechanics** → volumetric flow, shear force.
* **Process data analysis** → energy & cumulative balances.