Assignment 1

Problem 1 — Internal Energy Estimation With Non-Constant Heat Capacity

In a chemical process stream, an ideal gas is heated from 320 K to 820 K. However, its heat capacity varies significantly with temperature, following

$$c_v(T) = 700 + 0.35T - 2 \times 10^{-4} T^2 \quad \text{(J/kg·K)}.$$

Because the heater only measures temperature and flow, you must estimate the internal-energy rise numerically and examine how numerical integration accuracy depends on discretization.

- Compute the internal-energy change $\Delta u = \int_{T_1}^{T_2} c_v(T)\, dT$ using at least two MATLAB methods.
- Compare numerical results with the corresponding analytical expression obtained by symbolic integration.
- Determine the minimum grid resolution that keeps numerical error below 0.1%.

Hint: Use a vectorized anonymous function and compare `integral()`, `trapz()`, and symbolic `int()`.

Problem 2 — Energy Balance for a Closed System With Time-Varying Heating

A sealed reaction vessel undergoes an exothermic reaction while also receiving external heat. Internal energy depends on temperature via:

$$u(T) = 450 + 1.1T + 0.0012T^2 \quad \text{(kJ/kg)},$$

and the energy balance is:

$$\frac{du}{dt} = q_{\text{ext}}(t) + r(T),$$

with $q_{\text{ext}}(t) = 5000e^{-0.002t}$ kJ/s and $r(T) = 1500(1 - e^{-0.01T})$. Your task is to simulate internal-energy evolution and recover the temperature history.

- Integrate du/dt from 0–4000 s and compute the internal-energy profile.
- Convert $u(t)$ to $T(t)$ by numerically inverting the expression for $u(T)$.
- Find when reaction heat contribution surpasses external heating.

Hint: Integrate using `ode45` and invert $u(T)$ using `fsolve` or `interp1`.

Problem 3 — Entropy in a Compression Process With Real-Gas Effects

A gas is compressed from 1 bar to 20 bar along a polytropic path PV^n = constant with $n = 1.28$. Real-gas effects follow the analytic model:

$$Z(T, P) = 1 + 0.0008P - \frac{120}{T},$$

with $c_p = 1.05$ kJ/kg·K and $R = 0.287$. Entropy evolves as:

$$ds = c_p \frac{dT}{T} - R \frac{Z\, dP}{P}.$$

- Determine $T(P)$ along the polytropic path and evaluate the entropy change numerically.
- Compute the ideal-gas entropy change for comparison.
- Report percent deviation and discuss the influence of real-gas effects.

Hint: Compute $T(P)$ first, then evaluate the integral using `trapz` or `integral` on discretized data.

Problem 4 — Internal Energy and Entropy Tracking in an Open System

A steady-flow heater raises a gas stream from 310 K to 670 K. Thermodynamic properties follow:

$$h(T) = 300 + 2.5T + 0.0007T^2, \qquad s(T) = 2.0\ln(T) + 0.001T.$$

Energy and entropy balances:

$$\dot{Q} = \dot{m}(h_2 - h_1), \qquad \dot{S}_{gen} = \dot{m}(s_2 - s_1) - \frac{\dot{Q}}{T_b},$$

with $T_b = 300$ K.

- For $\dot{Q}$ from 20–100 kW, find all mass-flow values satisfying $\dot{S}_{gen} \geq 0$.
- Plot feasible $(\dot{Q}, \dot{m})$ regions.
- Explain the connection between internal-energy rise and the feasible operating zone.

Hint: Use `meshgrid` and logical indexing to filter allowed points.

Problem 5 — Exergy Analysis With Temperature-Dependent Properties

A stream is heated from 350 K to 900 K with a temperature-dependent heat capacity:

$$c_p(T) = 1200 + 0.4T - 1.2 \times 10^{-4}T^2.$$

Entropy change:

$$\Delta s = \int_{350}^{900} \frac{c_p(T)}{T}\, dT,$$

and exergy destruction is

$$\dot{X}_{dest} = T_0\, \dot{S}_{gen}, \quad T_0 = 298\,\text{K}.$$

- Compute Δs numerically.
- Estimate exergy destruction assuming heater irreversibility of 2% and 10%.
- Plot exergy destruction vs irreversibility level.

Hint: Use `integral()` with a vectorized $c_p(T)/T$ function.

Problem 6 — A Fully Dynamic Energy–Entropy Cycle Simulation

Boundary temperatures vary as:

$$T_h(t) = 900 - 300e^{-0.0008t}, \qquad T_c(t) = 300 + 40\sin(0.002t).$$

Efficiency:

$$\eta(t) = 1 - \frac{T_c(t)}{T_h(t)}.$$

Heat input:

$$Q_{in}(t) = 20000\,(1 + 0.3\sin(0.003t))\ \text{kW}.$$

- Compute work output $W(t)$ by numerically integrating $P(t) = \eta(t)Q_{in}(t)$.
- Evaluate entropy generation:

$$\dot{S}_{gen}(t) = \frac{Q_{in}(t)}{T_h(t)} - \frac{Q_{in}(t)}{T_c(t)}.$$

- Discuss how oscillations in both reservoir temperatures affect efficiency.

Hint: Use `trapz` over a finely spaced time grid.

Problem 7 — Polytropic Piston With Temperature-Dependent Internal Energy

A closed piston undergoes polytropic compression $PV^m = \text{const}$ with $m = 1.25$. State A: $P_A = 1$ bar, $T_A = 300$ K. State B: $P_B = 10$ bar. Internal energy:

$$u(T) = 500 + 0.8T + 1.5 \times 10^{-3}T^2\ \text{(kJ/kg)}.$$

Assume an ideal-gas relation with $R = 0.287$.

- Solve for the final temperature T_B using the polytropic relation.

- Compute $\Delta u = u(T_B) - u(T_A)$, heat, and work for the process.
- Compare numerical work with the analytical polytropic expression.

Hint: Use `fsolve` for T_B and `integral` for path work.

Problem 8 — Optimal Heating Profile Minimizing Entropy Generation

A material is heated from 300 K to 900 K over $t_f = 2000$ s. Temperature evolution: $c\dot{T} = q(t)$ with $c = 2.5$ kJ/K. Total heat input is fixed:

$$\int_0^{t_f} q(t)\, dt = 5 \times 10^5 \text{ kJ}.$$

Entropy generation:

$$\dot{s}_{gen}(t) = \frac{q(t)}{T(t)} - \frac{q(t)}{T_b}, \qquad T_b = 300\, K.$$

- Formulate the discrete optimization problem for minimizing total entropy generation.
- Solve using `fmincon` with the energy constraint.
- Compare the optimal profile with uniform heating.

Hint: Use a vector of decision variables $q_1, \ldots, q_N$ and include an equality constraint for total heat.

Problem 9 — Reaction Heat and Parameter Estimation Using Synthetic Data

Reaction heat is modeled as:

$$r(T) = Ae^{-E/(RT)}, \qquad R = 8.314 \times 10^{-3}.$$

Synthetic data must be generated by integrating

$$c\dot{T} = r(T) + 2000e^{-0.001t}, \qquad c = 1.8 \text{ kJ/K},$$

with true parameters $A = 1 \times 10^5$, $E = 45$ kJ/mol, then adding 1% noise.

- Generate noisy synthetic temperature–time data.
- Estimate A and E via `lsqcurvefit` or `fitnlm`.
- Discuss identifiability and effect of noise.

Hint: Wrap the ODE solver inside the objective function for parameter fitting.

Problem 10 — Entropy-Constrained Design of a Heat Pump Stage

Consider a heat pump transferring heat from 270 K to 320 K. Real COP:

$$\mathrm{COP}(r_p) = \frac{T_c}{T_h - T_c}\left(1 - \alpha\frac{(r_p - 1)^2}{r_p}\right), \quad \alpha = 0.02.$$

Compressor work:

$$W_c = k(r_p^{0.5} - 1), \qquad k = 50.$$

- Determine the pressure ratio $r_p \in [1.1, 6]$ that maximizes heat delivered per unit work, subject to entropy generation < 0.05 kJ/K.
- Produce contour and 1-D plots of COP, entropy generation, and the feasible region.
- Explain trade-offs between higher pressure ratio and entropy generation.

Hint: Use `fmincon` with a nonlinear inequality constraint.