Title: Q2: PFR – Cracking of Acetone

Reaction and kinetics

- Reaction: CH_3COCH_3 (A) → CH_2CO (B) + CH_4 (C)
- Irreversible vapor-phase cracking in an adiabatic plug-flow reactor.
- First order in acetone: $-r_A = k\,C_A$
- Rate constant: $\ln k\ (s^{-1}) = 34.34 - 34222/T\ (K)$
- Gas-phase concentration: $C_A\ (mol/m^3) = 1000\, y_A P / (R T)$

Thermochemistry

- Enthalpy of reaction (J/mol) as a function of T (K):
  $\Delta H = 80770 + 6.8\,(T - 298) - 0.00575\,(T^2 - 298^2) - 1.27\times10^{-6}\,(T^3 - 298^3)$
- Heat capacities (J/mol·K):
  $C_{pA} = 26.2 + 0.183\,T - 45.86\times10^{-6}\,T^2$
  $C_{pB} = 20.04 + 0.0945\,T - 30.95\times10^{-6}\,T^2$
  $C_{pC} = 13.39 + 0.077\,T - 18.91\times10^{-6}\,T^2$

Reactor and operating data

- Acetone feed: 8000 kg/h = 38.3 gmol/s (max reactor capacity)
- Inlet temperature: $T_0 = 1150$ K (unless stated otherwise)
- Pressure: P = 162 kPa (1.6 atm) unless varied
- Reactor volume: V = 4 m^3
- Products at outlet: ketene, methane; unreacted acetone; possible N_2 diluent.

Tasks

I. For acetone-only feed (38.3 gmol/s), calculate:

1. Outlet molar flow rate (gmol/s)
2. Mole fraction of each species at the reactor outlet
   Conditions: adiabatic PFR, P = 162 kPa, V = 4 m^3, T_0 = 1150 K.

II. To increase conversion, feed nitrogen with acetone while keeping total molar feed at 38.3 gmol/s. For N_2 feed rates of 28.3, 18.3, 8.3, 3.3, and 0.0 gmol/s:

- Compute final conversions and outlet temperatures as a function of reactor volume.
- Use C_{p,N_2} (J/mol·K): $6.25 + 0.008787\,T - 2.1\times10^{-8}\,T^2$.
- Plot conversion vs reactor volume and temperature vs reactor volume.

III. Vary pressure and acetone feed. For $1.6\text{ atm} \le P \le 5\text{ atm}$ and acetone feed rates F_{A0} of 10, 20, 30, 35, and 38.3 gmol/s (with N_2 co-fed to keep total feed 38.3 gmol/s, inlet $T = 1035$ K):

- Calculate final conversion and outlet temperature for each case.
- Plot final conversion vs P and F_{A0}; plot final temperature vs P and F_{A0}.

Notes

- Treat the reactor as adiabatic PFR with variable temperature and density.
- Use ideal-gas behavior for concentration via $C_A = 1000\, y_A P/(R\,T)$.