

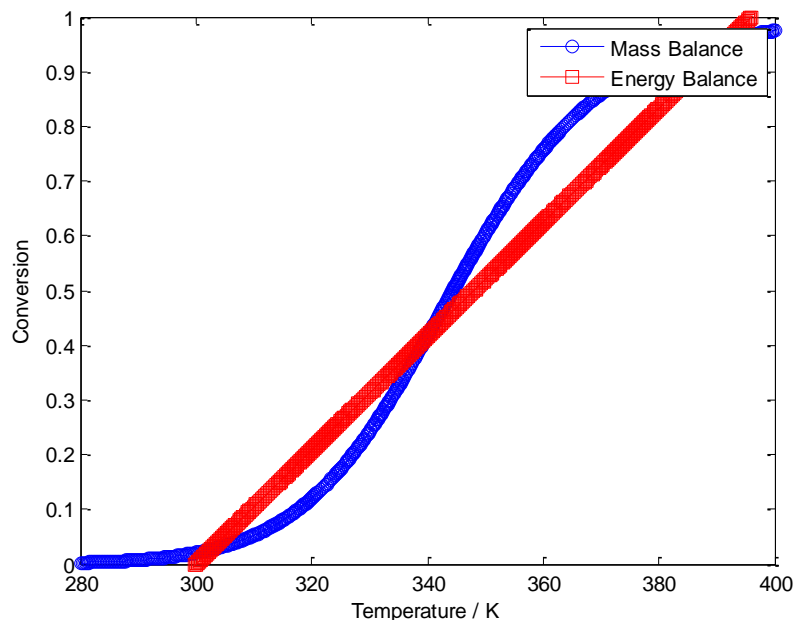
Multiple steady states of a CSTR

Consider the production of propylene glycol (C) in an adiabatic CSTR. Initially there is only 2 kmol/m³ propylene oxide (A) present in the 1.25 m³ reactor at temperature T₀. The feed stream consists of 20 kmol/h propylene oxide, 200 kmol/h water (B) containing 0.1 wt% sulphuric acid, and 33 kmol/h of methanol (inert material). Calculate the properties of water directly without accounting for the presence of sulphuric acid.

Data: $F_{A-in} = 20$ kmol/h, $F_{B-in} = 200$ kmol/h, $F_{M-in} = 33$ kmol/h, $C_{pA} = 120$ J/mol/K, $C_{pB} = 60$ J/mol/K, $C_{pM} = 60$ J/mol/K, $C_{pC} = 100$ J/mol/K, ΔH_{Rxn} at 20 °C = -85000 J/mol of A reacted. Feed temperature = 27 °C (after accounting for heat of mixing), $k = 17 \times 10^{11} e^{\frac{-9000}{T}}$ h⁻¹ where T is in K.

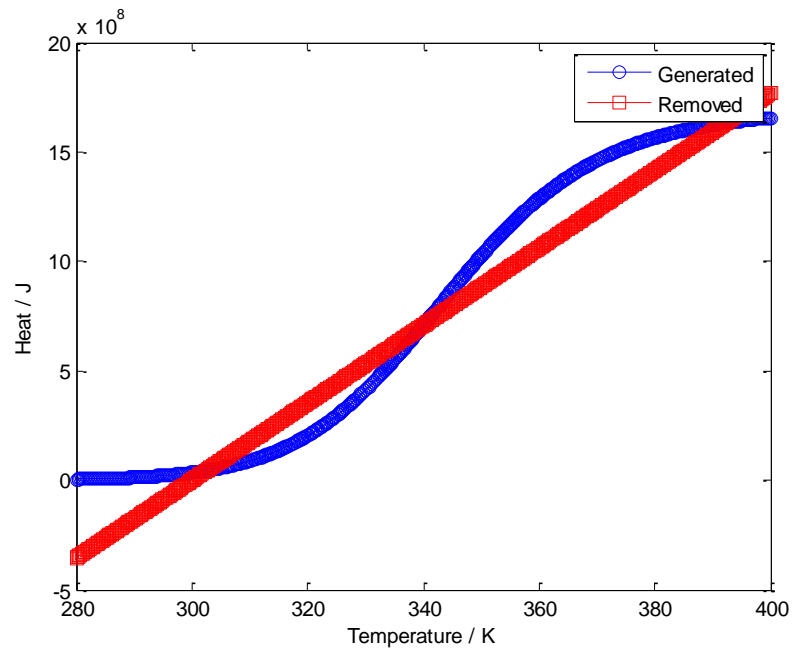
The volumetric flow rates of methanol and propylene oxide were 1.5 kL/h each and that of water is 6.5 kL/h. $Q_{in} = 9.5$ kL/h. The CSTR volume is 1.25 kL.

- By application of the material and energy balances, determine the possible steady state exit concentration/conversion and temperature for the glass lined reactor.
(There are a number of ways to solve the material and energy balance equations. However, to get insight into the functional relationship between X (Conversion) and reactor temperature (T), use a graphical solution. X could be plotted as a function of T for the mole and energy balances, and the intersection of the two curves gives the solution where both the mole and energy balance solutions are satisfied. In addition, by plotting these two curves you can also see if there are more than one intersection (i.e. multiple steady states) for which both the energy balance and mole balance are satisfied.)



Thus all the three solutions are possible.

- 2) To study the multiplicity of steady states, plot heat generation ($G(T)$) and heat removal ($R(T)$) curves as a function of temperature and analyse the stability of all the steady states obtained.

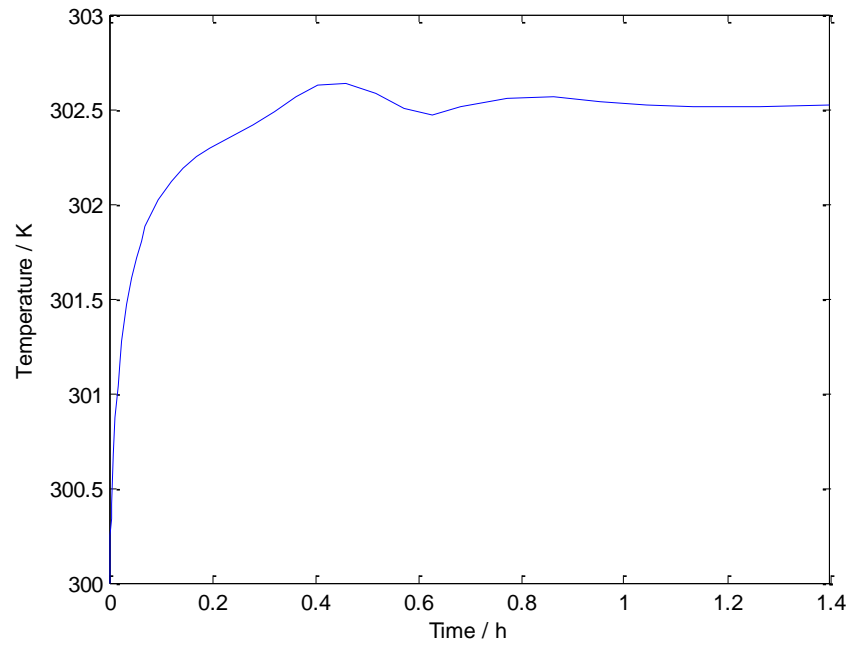


At the intermediate level a slight increase in temperature will produce more conversion (since heat generation is more than the heat removal) which in turn will increase the temperature and it will end up at the high conversion.

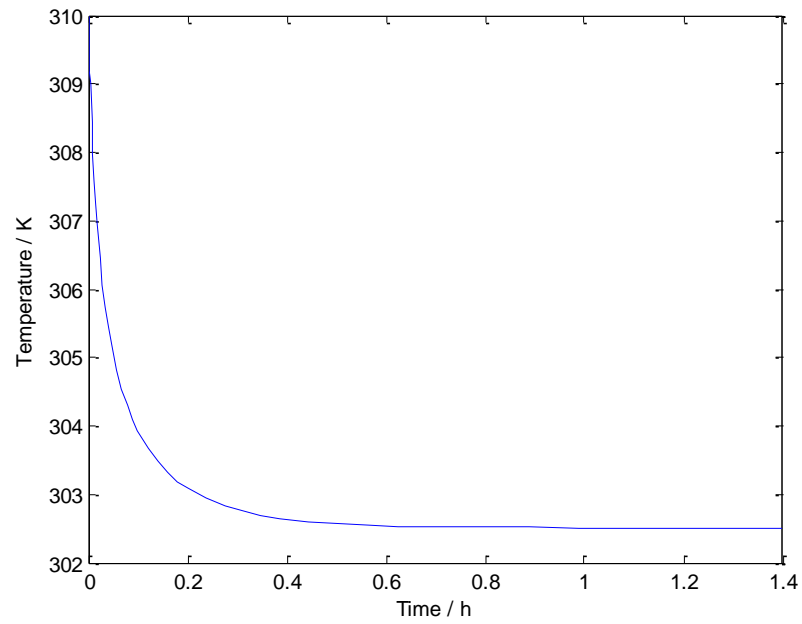
At the low end, an increase in temperature will cause a slight increase in heat generation but more of it will be removed by the outgoing fluid (heat removal), so the temperature will decrease and come back to original steady state value. Similar argument holds for high temperature steady state also.

- 3) Verify the region of stability and instability by simulating the reactor startup to see how temperature and concentration approach their steady state values. This could be done by solving the unsteady temperature-time and concentration-time equations numerically.

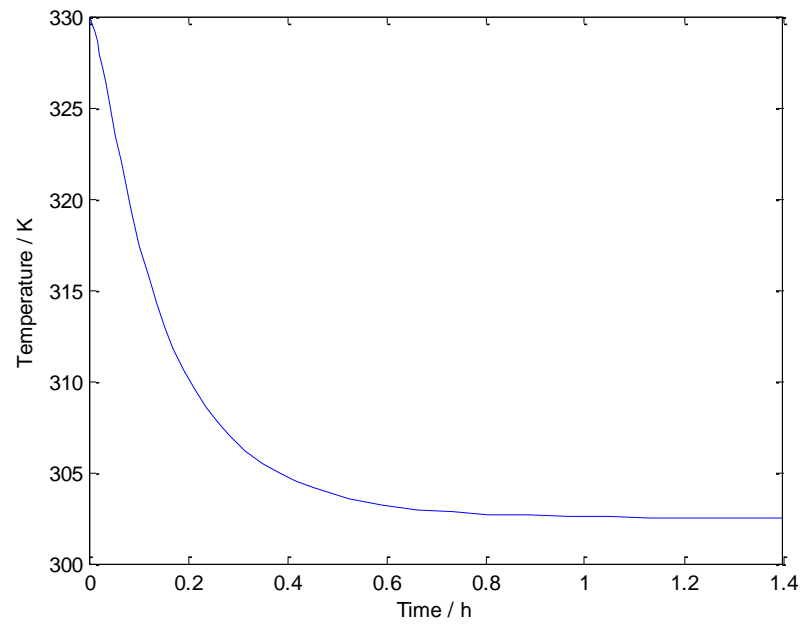
a) $T_0 = 300 \text{ K}$



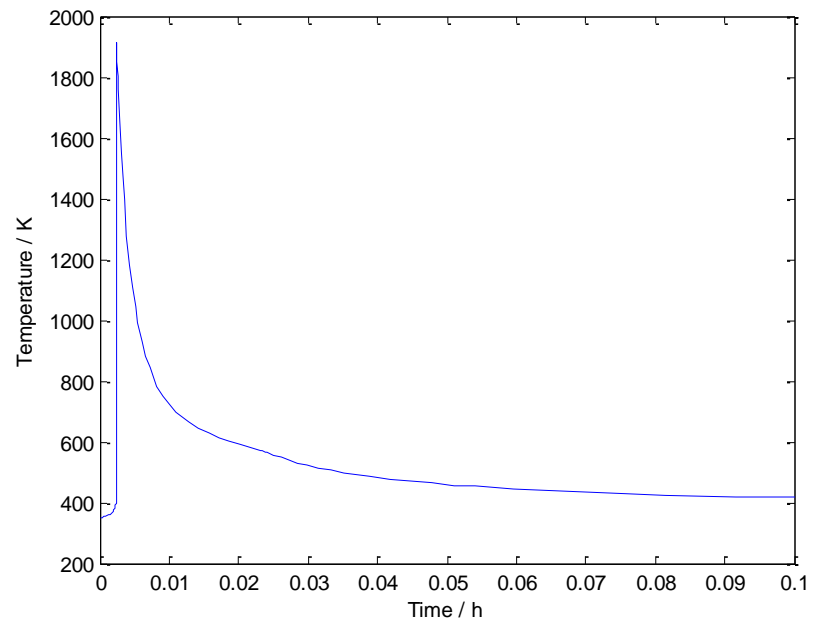
b) $T_0 = 310 \text{ K}$



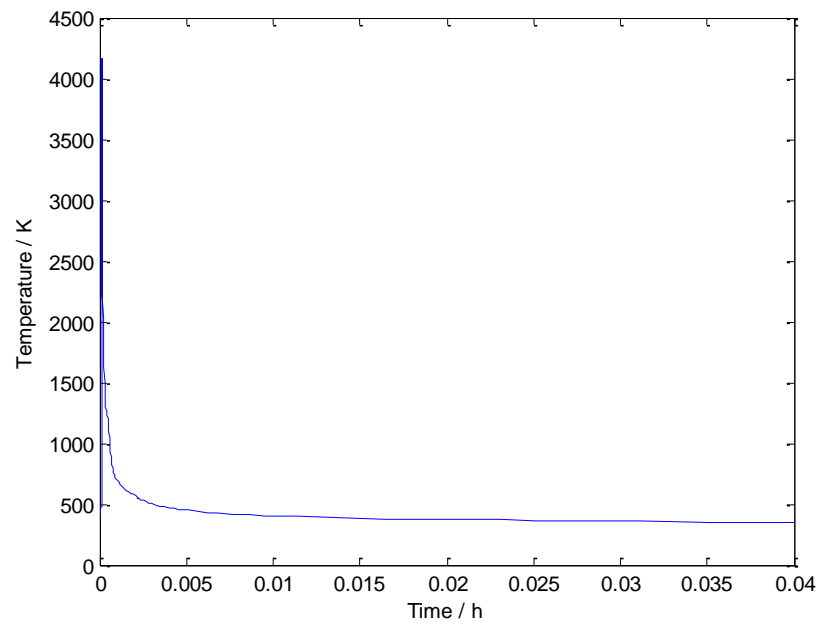
c) $T_0 = 330 \text{ K}$



d) $T_0 = 350 \text{ K}$



e) $T_0 = 400 \text{ K}$



Steady State CSTR design Algorithm

Algorithm

Example: Elementary irreversible liquid-phase reaction
 $A \rightarrow B$ Given $F_{A0}, C_{A0}, k_0, E, C_{pi}, H_i^\circ$

CSTR

Design equation $V = \frac{F_{A0}X}{-r_A}$
 Rate law $-r_A = kC_A$
 Stoichiometry $C_A = C_{A0}(1-X)$
 Combining $V = \frac{F_{A0}X}{kC_{A0}(1-X)}$

X specified:
calculate V and T

V specified:
calculate X and T

Need $k(T)$

Calculate T

$$T = \frac{X[-\Delta H_{RX}^\circ(T_R)] + \sum \theta_i \tilde{C}_{pi} T_0 + X \Delta \hat{C}_p T_R}{\sum \theta_i \tilde{C}_{pi} + X \Delta \hat{C}_p}$$

Calculate k

$$k(T) = k_0 \exp \left[\frac{E}{R} \left(\frac{1}{T_0} - \frac{1}{T} \right) \right]$$

Calculate V

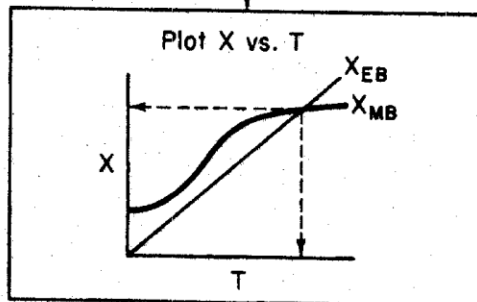
$$V = \frac{F_{A0}X}{kC_{A0}(1-X)}$$

Two equations and two unknowns

$$X_{MB} = \frac{\tau k}{1 + \tau k}, \tau = \frac{VC_{A0}}{F_{A0}}$$

$$X_{MB} = \frac{\tau A e^{-E/RT}}{1 + \tau A e^{-E/RT}}$$

$$X_{EB} = \frac{\frac{UA(T-T_0)}{F_{A0}} + \sum \theta_i \tilde{C}_{pi} (T - T_0)}{-[\Delta H_R^\circ(T_R) + \Delta \hat{C}_p (T - T_R)]}$$



Heat removal and heat generation terms

$$G(T) = (-\Delta H_{\text{Rx}}^{\circ})(-r_A V / F_{A0})$$

$$R(T) = C_{p0}(1 + \kappa)(T - T_c)$$

Unsteady state mole and energy balances for a CSTR

Mole balances:

		Initial Conditions
A:	$\frac{dC_A}{dt} = r_A + \frac{(C_{A0} - C_A)v_0}{V}$	0
B:	$\frac{dC_B}{dt} = r_B + \frac{(C_{B0} - C_B)v_0}{V}$	$C_{Bi} = 3.45 \frac{\text{lb mol}}{\text{ft}^3}$
C:	$\frac{dC_C}{dt} = r_C + \frac{-C_C v_0}{V}$	0
M:	$\frac{dC_M}{dt} = \frac{v_0(C_{M0} - C_M)}{V}$	0

Rate law:

$$-r_A = kC_A$$

Stoichiometry:

$$-r_A = -r_B = r_C$$

Energy balance:

$$\frac{dT}{dt} = \frac{Q - F_{A0} \sum \Theta_i C_{pi}(T - T_0) + (\Delta H_{\text{Rx}})(r_A V)}{\sum N_i C_{pi}}$$