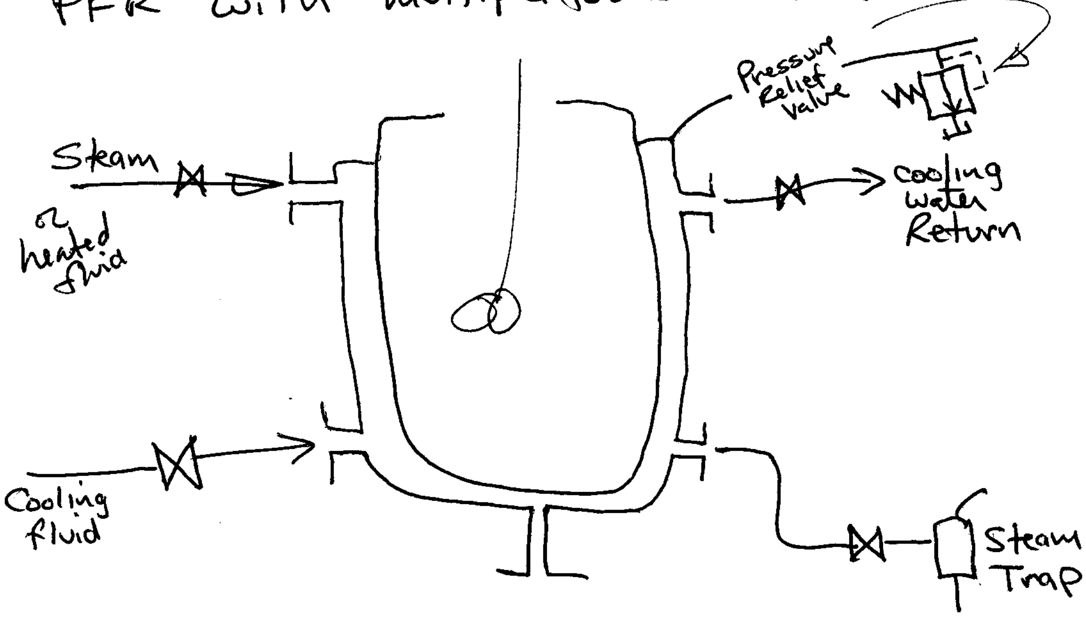
Chapter 8

Show pictures of

CSTR with jacket

PFR with multiple tubes & shell



Typical values for steam heating of water

$U = 70$ Btu/hr ft²°F water

$U = 55$ Btu/hr ft²°F Toluene

90 RPM

Best scenario is to use a single heat transfer fluid for both heating and cooling

Dowtherm $\underbrace{-80 - 315}_{J}$°C or $\overbrace{15 - 400}^{A}$°C

Syltherm $-100 - 260$°C

Typical values for shell & tube - see Perry's

What happens if we use saturated steam?

at 30 psia 250°F

15 psia 212 F (atmospheric)

this keeps a constant temperature in jacket.

Ch 8

Why do we need a detailed E bal?

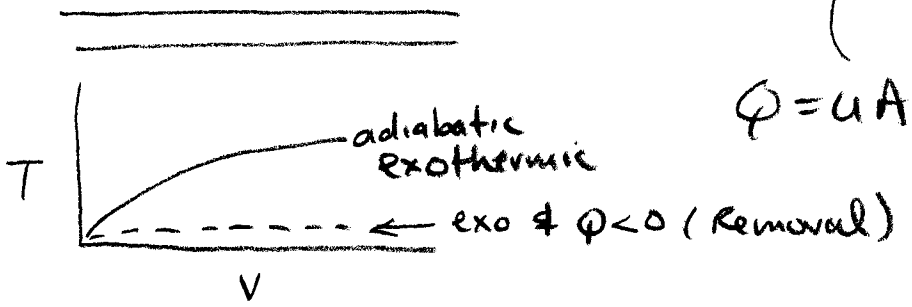
overall mol balance $\quad \chi = \dfrac{F_{i0} - F_i}{F_{i0}}$

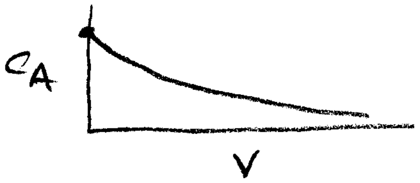
overall E balance

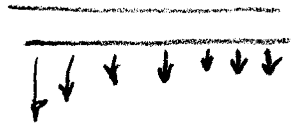
$$0 = \sum F_{i_0} H_{i_0} - \sum F_i H_i + \dot{Q}$$

heat in as positive

$$Q = UA(T_a - T)$$







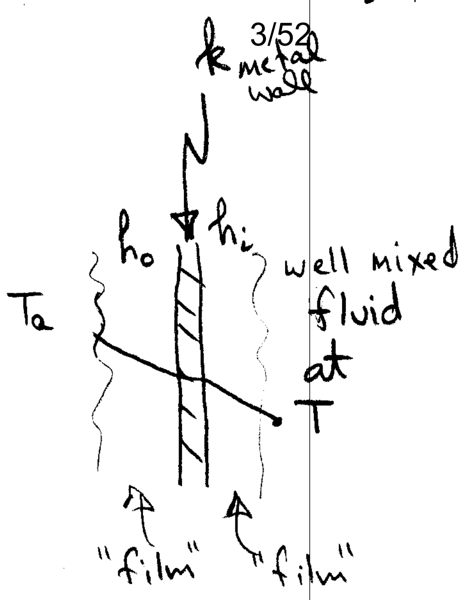
$r = -kC_A$

$k = A\exp(-E/RT)$

from E Bal

Chapter 8 -

heat added by jacket

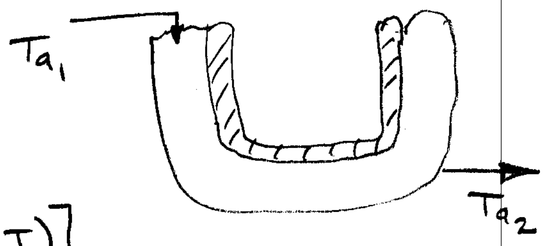


CASE I — $\dot{Q} = U_i A_i (T_a - T)$ (8-34)

$$\frac{1}{U_i} = \frac{1}{h_i} + \frac{\Delta x A_i}{k A_o} + \frac{1}{h_o}\frac{A_i}{A_o}$$

$\Delta T_a \cong 0$ — ① fast flow of liquid
② condensing steam

CASE II
If T_a changes then use a ΔT_{lnmean}



$\dot{Q} = U A_i \Delta T_{lm}$

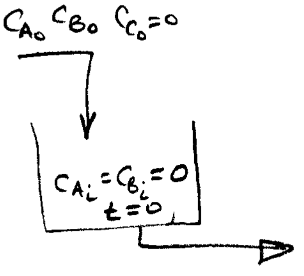
(8-35) $$\Delta T_{lm} = \frac{T_{a_1} - T_{a_2}}{\ln[(T_{a_1} - T)/(T_{a_2} - T)]}$$

$\boxed{8-61}$
$$V \sum_{i=1}^{n} C_{p_i} C_i \frac{dT}{dt} = \boxed{\overset{\dot{Q}}{U_i A_i (T_a - T)}} - \dot{W}_s - F_{A0} \sum_{i=1}^{n} \frac{F_{i0}}{F_{A0}} \tilde{C}_{p_i} (T - T_{i0})$$
$$- \Delta H_{Rxn}\Big|_T (-r_A V)$$

for more than one reaction
$$\sum_{j=1}^{m} \Delta H_{Rxn_j}\Big|_T (-r_{ij} V)$$

$$A + B \rightarrow C$$

① Assume that $C_{A0} \neq 0$ & $C_{B0} \neq 0$ $C_{C0} = 0$
② Same T



$$V \left[C_{p_A} C_A + C_{p_B} C_B + C_{p_C} C_C \right] \frac{dT}{dt}$$

$$= U_i A_i (T_a - T) - \dot{W}_s - F_{A0} \left[\frac{F_{A0}}{F_{A0}} \tilde{C}_{p_A} + \frac{F_{B0}}{F_{A0}} \tilde{C}_{p_B} + \cancelto{0}{\frac{F_{C0}}{F_{A0}}} \tilde{C}_{p_C} \right] (\overset{\text{out}}{T} - \overset{\text{in}}{T_0}) + \Delta H_{rxn} \, {-r_A V}$$

But Remember definitions

$$\tilde{C}_{P_i} \equiv \frac{\int_{T_0}^{T} C_{P_i}\, dT}{T - T_0}$$

entering fluid Temperature

(fluidized bed Highly exot

fixed bed: $\Delta H = -40 \frac{\text{kcal}}{\text{mol}}$

AND

$$\Delta H_{Rxn}\Big|_T = \Delta H^\circ_{Rxn}\Big|_{T_R} + \Delta\hat{C}_p (T - T_R) \qquad (8\text{-}27)$$

per mole or kg of A.

must be the same

Reference temperature (eg. $T_R = 298\text{ K}$) or 20°C

$$\Delta\hat{C}_p \equiv \frac{\int_{T_R}^{T} \Delta C_p\, dT}{T - T_R}$$

$$\Delta C_p \equiv \frac{d}{a} C_{P_D} + \frac{c}{a} C_{P_C} - \frac{b}{a} C_{P_B} - \frac{a}{a} C_{P_A}$$

per mole or kg of A!

Don't forget to include any $\Delta H_{\text{melting}}$ or $\Delta H_{\text{vaporization}}$!

See example 8-2

$\Delta H^\circ_{Rxn}\Big|_{T_R} \rightarrow$ See 8-24

Effect of P see bottom of page 391!

Energy Balance Derivations

Evaluating the work term: 8.2.2: The work term is given by flow work plus mechanical work:

$$\dot{W} = -\sum_{i=1}^{n} F_i PV\Big|_{in} + \sum_{i=1}^{n} F_i PV\Big|_{out} + \dot{W}_s \qquad (1)$$

CSTR Energy Balance

Control Volume: Fluid inside the reactor

Assumptions: The fluid is perfectly mixed - temperature of fluid is uniform

1) No ΔH_{rxn}
2) C_p's are integral averages

Mole Balance:

$$\frac{dN_i}{dt} = F_{i0} - F_i + \frac{\nu_i}{-a} r_A V \quad E.B \qquad (2)$$

The steady-state mole balance is:

$$F_i = F_{i0} + \frac{\nu_i}{-a} r_A V \quad M.B. \qquad (3)$$

Energy Balance:

Accumulation = in - out + generation

work done by system on surroundings

$$\frac{d\overline{HN}}{dt} = \sum_{i=1}^{n} H_{i0} F_{i0} - \sum_{i=1}^{n} H_i F_i + \dot{Q} - \dot{W}_s \qquad (4)$$

Basic Balance – Same form as Felder

For steady-state operation:

$$0 = \sum_{i=1}^{n} H_{i0} F_{i0} - \sum_{i=1}^{n} H_i F_i + \dot{Q} - \dot{W}_s \qquad (5)$$

Using a mean heat capacity, $\widetilde{C}_{pi}$, of species i between temperature $T0$ and temperature T

To is inlet reactor feed Temp.

$$\widetilde{C}_{pi} \equiv \frac{\int_{T_0}^{T} C_{pi}\,dT}{T - T_0} \qquad (6)$$

Definition given on Exam Page

the species enthalpy can be defined as

$$H_i = H_{i0} + \widetilde{C}_{pi}(T - T_0) \qquad (7)$$

F_i = eqn 3

Inserting the enthalpy defined by equation 7 and the steady-state mole balance of equation 3 yields:

$$0 = \sum_{i=1}^{n} H_{i0} F_{i0} - \sum_{i=1}^{n} \underbrace{\left(H_{i0} + \widetilde{C}_{pi}(T - T_0)\right)}_{H_i\ \text{eqn (7)}} \left(F_{i0} + \frac{\nu_i}{-a} r_A V\right) + \dot{Q} - \dot{W}_s \qquad (8)$$

multiply out terms

$$0 = \sum_{i=1}^{n} H_{i0} F_{i0} - \sum_{i=1}^{n} H_{i0} F_{i0} - \sum_{i=1}^{n} \left(F_{i0} \widetilde{C}_{pi}(T - T_0)\right) + \sum_{i=1}^{n} \left(\frac{\nu_i}{a} H_{i0} + \frac{\nu_i}{a} \widetilde{C}_{pi}(T - T_0)\right)(r_A V) + \dot{Q} - \dot{W}_s \qquad (9)$$

Using the definition of the heat of reaction, $\Delta H_{rxn}|_{T_0}$, and an overall change in heat capacity, $\Delta\widetilde{C}_{pi}$,

group $\Delta H_{rxn}\backslash T_0$

$$\Delta H_{rxn}|_{T_0} = \frac{d}{a} H_D|_{T_0} + \frac{c}{a} H_C|_{T_0} - \frac{b}{a} H_B|_{T_0} - H_A|_{T_0} = \sum_{i=1}^{n} \frac{\nu_i}{a} H_i|_{T_0}$$

with

$$\Delta\widetilde{C}_p = \frac{d}{a}\widetilde{C}_{pD} + \frac{c}{a}\widetilde{C}_{pC} - \frac{b}{a}\widetilde{C}_{pB} - \widetilde{C}_{pA} = \sum_{i=1}^{n} \frac{\nu_i}{a} \widetilde{C}_{pi} \qquad (10)$$

the CSTR energy balance is:

$$0 = -\sum_{i=1}^{n} \left(F_{i0} \widetilde{C}_{pi}(T - T_0)\right) + \left(\Delta H_{rxn}|_{T_0} + \Delta\widetilde{C}_{pi}(T - T_0)\right)(r_A V) + \dot{Q} - \dot{W}_s \qquad (11)$$

and finally using the heat of reaction at the fluid temperature, $\Delta H_{rxn}|_T$

group $\Delta H_{rxn}\backslash T$

$$\Delta H_{rxn}|_T = \Delta H^{\circ}_{rxn}|_{T_0} + \Delta\widetilde{C}_p (T - T_0)$$

gives the following steady-state mole balance for a CSTR:

$$0 = -\sum_{i=1}^{n} \left(F_{i0} \widetilde{C}_{pi}(T - T_0)\right) + \left(\Delta H_{rxn}|_T\right)(r_A V) + \dot{Q} - \dot{W}_s \qquad (12)$$

$$0 = \underbrace{F_{A0} - F_A}_{F_{A0}x} + r_A V \qquad -F_{A0}X = +r_A V$$

Now it is eqn 8-48

1) Show that balance has no ΔH_{rxn}

2) Define ΔH_{rxn}

3) Cp's are raw data & not averages

Energy Balance Derivation: PFR

Control Volume: a small cylindrical volume of fluid (plug) ΔV

Assumptions: There are no gradients of T, P, and C_i within the control volume with respect to r and θ.

Mole Balance:
$$\frac{\partial C_i}{\partial t} = -\frac{\partial F_i}{\partial V} + \frac{\nu_i}{-a} r_A \tag{1}$$

The steady-state mole balance is:
$$\frac{\mathrm{d}F_i}{\mathrm{d}V} = \frac{\nu_i}{-a} r_A \tag{2}$$

Energy Balance:

Accumulation = in - out + generation

No ΔH_{rxn}?

Balance

$$\frac{\mathrm{d}\overline{HC}}{\mathrm{d}t}\Delta V = \sum_{i=1}^{n} H_iF_i\Big|_V - \sum_{i=1}^{n} H_iF_i\Big|_{V+\Delta V} + \dot{q}\Delta V - \dot{w}_s\Delta V \tag{3}$$

↓

divide by ΔV

$$\frac{\mathrm{d}\overline{HC}}{\mathrm{d}t} = \frac{-\left(\sum_{i=1}^{n} H_iF_i\Big|_{V+\Delta V} - \sum_{i=1}^{n} H_iF_i\Big|_V\right)}{V+\Delta V - V} + \dot{q} - \dot{w}_s \tag{4}$$

↓

lim ΔV→0

$$\lim_{\Delta V\to 0}\left[\frac{\mathrm{d}\overline{HC}}{\mathrm{d}t} = \frac{-\left(\sum_{i=1}^{n} H_iF_i\,{}_i\Big|_{V+\Delta V} - \sum_{i=1}^{n} H_iF_i\Big|_V\right)}{V+\Delta V - V} + \dot{q} - \dot{w}_s\right] \tag{5}$$

Final Equation →

$$\boxed{\frac{\partial\overline{HC}}{\partial t} = \frac{-\partial\left(\sum_{i=1}^{n} H_iF_i\right)}{\partial V} + \dot{q} - \dot{w}_s} \quad \text{No } \Delta H_{rxn} \tag{6}$$

SS For steady-state operation:

$$\boxed{\text{mistake}} \rightarrow \frac{+\mathrm{d}\left(\sum_{i=1}^{n} H_iF_i\right)}{\mathrm{d}V} = \dot{q} - \dot{w}_s \quad \text{No } \Delta H_{rxn} \tag{7}$$

<u>Using the chain rule</u>:

$$\sum_{i=1}^{n}\left[H_i\boxed{\frac{\mathrm{d}F_i}{\mathrm{d}V}} + F_i\frac{\mathrm{d}H_i}{\mathrm{d}V}\right] = \dot{q} - \dot{w}_s \tag{8}$$

put in mole balance for each species

Substituting the steady-state mole balance from equation 2 into the heat balance to eliminate $\frac{\mathrm{d}F_i}{\mathrm{d}V}$

Now we have a reaction term

↓

$$\sum_{i=1}^{n}\left[H_i\frac{\nu_i}{-a} r_A + F_i\frac{\mathrm{d}H_i}{\mathrm{d}V}\right] = \dot{q} - \dot{w}_s \tag{9}$$

$$\sum_{i=1}^{n}\left[F_i\frac{\mathrm{d}H_i}{\mathrm{d}V}\right] = \sum_{i=1}^{n}\left[H_i\frac{\nu_i}{a} r_A\right] + \dot{q} - \dot{w}_s \tag{10}$$

Starting to look familiar

Using the definition of the heat of reaction, $\Delta H_{rxn}\big|_T$

$\Delta H_{rxn}\big|_T$ definition

$$\Delta H_{rxn}\big|_T = \frac{d}{a}H_D\big|_T + \frac{c}{a}H_C\big|_T - \frac{b}{a}H_B\big|_T - H_A\big|_T = \sum_{i=1}^{n}\frac{\nu_i}{a}H_i\big|_T \tag{11}$$

$$\sum_{i=1}^{n}\left[F_i\frac{\mathrm{d}H_i}{\mathrm{d}V}\right] = \Delta H_{rxn}\big|_T r_A + \dot{q} - \dot{w}_s \tag{12}$$

Substituting the definition of the enthalpy: $H_i = C_{pi}T$ ← look at Cp's they are not integral averages

$$\sum_{i=1}^{n}\left[F_iC_{pi}\right]\frac{\mathrm{d}T}{\mathrm{d}V} = \Delta H_{rxn}\big|_T r_A + \dot{q} - \dot{w}_s \tag{13}$$

Substituting in for the molar flowrate of species i defined from chemical equation stoichiometry:

8-35 $\dfrac{dT}{dV} = \dfrac{\Delta H_{rxn} r + \dot{q}}{\Sigma F_i C_{p_i}} \rightarrow$

$$\frac{\mathrm{d}T}{\mathrm{d}V} = \frac{\Delta H_{rxn}\big|_T r_A + \dot{q} - \dot{w}_s}{\sum_{i=1}^{n}\left[\left(F_{i0} + \frac{\nu_i}{a}F_{A0}\chi_A\right)C_{pi}\right]} \tag{14}$$

And using Foglers notation for the the change in heat capacity, ΔC_{pi},

with
$$\Delta C_p = \frac{d}{a}C_{pD} + \frac{c}{a}C_{pC} - \frac{b}{a}C_{pB} - C_{pA} = \sum_{i=1}^{n}\frac{\nu_i}{a}C_{pi} \tag{15}$$

$$\frac{\mathrm{d}T}{\mathrm{d}V} = \frac{\Delta H_{rxn}\big|_T r_A + \dot{q} - \dot{w}_s}{\sum_{i=1}^{n}F_{i0}C_{pi} + \Delta C_p F_{A0}\chi_A} \tag{16}$$

This is the Fogler equation 8-54 similar to (In form)

Standard definition Equation 8-27

Not $\Delta H_{rxn}\big|_T = \Delta H^\circ_{RXN}\big|_{T_R} + \Delta\hat{C}_p\,(T - T_R)$

Note that this term will have some sort of integral average

$$\left\{\ \hat{C}_p \equiv \frac{\int_{T_R}^{T} C_p\,dT}{T - T_R}\right.$$

alternative

ENERGY BALANCE Derivations: Batch Reactors:

Control Volume: Fluid inside the reactor
Assumptions: The fluid is perfectly mixed - temperature of fluid is uniform

Mole Balance:
$$\frac{dN_i}{dt} = \frac{\nu_i}{-a} r_A V \tag{1}$$

Energy Balance:
Accumulation = in - out + generation

Basic Balance
$$\frac{d\overline{E}N}{dt} = \frac{d\left(\overline{U} + \overline{KE} + \overline{PE}\right)N}{dt} = \dot{Q} - \dot{W} \tag{2}$$

For most chemical reactor situations the kinetic, $\overline{KE}$, and potential energy, $\overline{PE}$, terms are negligible compared to the internal energy term, $\overline{U}$. In addition, the internal energy is given by
$$\overline{U} = \overline{H} - PV \tag{3}$$

Two derivations are given below; one for liquids and the other for gases.

Batch Reactors (Closed systems)

Liquid Derivation:

For liquids the internal energy is approximately equal to the enthalpy

→ Great Assumption: $\overline{U} \approx \overline{H}$ (4)

Substituting equation 13 and assuming that the internal energy is equal to the total energy yields:

B
$$\frac{d}{dt}\left[\overline{H}N\right] = \frac{d}{dt}\left[\left(\sum_{i=1}^{n} N_i H_i\right)\right] = \sum_{i=1}^{n}\left[H_i \frac{dN_i}{dt} + N_i \frac{dH_i}{dt}\right] = \dot{Q} - \dot{W}_s \tag{5}$$

Using the batch reactor mole balance, equation (1), into equation (5) to eliminate $\frac{dN_i}{dt}$ gives:

$$\sum_{i=1}^{n}\left[\left(\frac{\nu_i}{-a} r_A V\right) H_i + N_i \frac{dH_i}{dt}\right] = \dot{Q} - \dot{W}_s \tag{6}$$

$$\sum_{i=1}^{n}\left[N_i \frac{dH_i}{dt}\right] = \sum_{i=1}^{n}\left[\left(\frac{\nu_i}{a} r_A V\right) H_i\right] + \dot{Q} - \dot{W}_s = \sum_{i=1}^{n}\left(\frac{\nu_i}{a} H_i\right) r_A V + \dot{Q} - \dot{W}_s \tag{7}$$

The definition of the heat of reaction at a temperature, T, is:

$$\Delta H_{rxn}\big|_T = \frac{d}{a} H_D\big|_T + \frac{c}{a} H_C\big|_T - \frac{b}{a} H_B\big|_T - H_A\big|_T = \sum_{i=1}^{n} \frac{\nu_i}{a} H_i\big|_T \tag{8}$$

$$\sum_{i=1}^{n}\left[N_i \frac{dH_i}{dt}\right] = \Delta H_{rxn}\big|_T r_A V + \dot{Q} - \dot{W}_s \tag{9}$$

Since $H_i = C_{pi} T$ and from the stoichiometric table $N_i = N_{i0} + \frac{\nu_i}{a} N_{A0} \chi_A$

$$\sum_{i=1}^{n}\left[C_{pi}\left(N_{i0} + \frac{\nu_i}{a} N_{A0} \chi_A\right)\right]\frac{dT}{dt} = \Delta H_{rxn}\big|_T r_A V + \dot{Q} - \dot{W}_s \tag{10}$$

Using Foglers notation:

$$\sum_{i=1}^{n}\left[C_{pi} N_{i0} + \Delta C_p N_{A0} \chi_A\right]\frac{dT}{dt} = \Delta H_{rxn}\big|_T r_A V + \dot{Q} - \dot{W}_s \tag{11}$$

Batch equation

with
$$\Delta C_p = \frac{d}{a} C_{pD} + \frac{c}{a} C_{pC} - \frac{b}{a} C_{pB} - C_{pA} \tag{12}$$

Do the ~~type~~ Same things

GAS

Gas Derivation

For gases the internal energy is given by equation 3 and substituting the ideal gas law yields:

$$\overline{U}=\overline{H}-\overline{PV}=\overline{H}-RT \tag{13}$$

Substituting equation 13 into equation 5 and assuming that the internal energy is equal to the

Using the batch reactor mole balance, equation (1), into equation (14) to eliminate $\frac{dN_i}{dt}$ gives:

$$\sum_{i=1}^{n}\left[\left(\frac{\nu_i}{-a}r_AV\right)(H_i-RT)+N_i\frac{dH_i}{dt}-RN_i\frac{dT}{dt}\right]=\dot{Q}-\dot{W}_s \tag{15}$$

$$\sum_{i=1}^{n}\left[N_i\frac{dH_i}{dt}-RN_i\frac{dT}{dt}\right]=\sum_{i=1}^{n}\left(\frac{\nu_i}{a}(H_i-RT)\right)r_AV+\dot{Q}-\dot{W}_s \tag{16}$$

The definition of the heat of reaction at a temperature, T, is:

$$\Delta H_{rxn}\big|_T=\frac{d}{a}H_D\big|_T+\frac{c}{a}H_C\big|_T-\frac{b}{a}H_B\big|_T-H_A\big|_T=\sum_{i=1}^{n}\frac{\nu_i}{a}H_i\big|_T \tag{17}$$

$$\sum_{i=1}^{n}\left[N_i\frac{dH_i}{dt}\right]=\Delta H_{rxn}\big|_T r_AV+\sum_{i=1}^{n}\left(-RT\frac{\nu_i}{a}\right)r_AV+\dot{Q}-\dot{W}_s \tag{18}$$

Since $H_i=C_{pi}T$ and from the stoichiometric table $N_i=N_{i0}+\frac{\nu_i}{a}N_{A0}\chi_A$

$$\sum_{i=1}^{n}\left[(C_{pi}-R)\left(N_{i0}+\frac{\nu_i}{a}N_{A0}\chi_A\right)\right]\frac{dT}{dt}=\Delta H_{rxn}\big|_T r_AV+\sum_{i=1}^{n}\left(-RT\frac{\nu_i}{a}\right)r_AV+\dot{Q}-\dot{W}_s \tag{19}$$

Using Foglers notation:

$$\sum_{i=1}^{n}[C_{vi}N_{i0}+\Delta C_vN_{A0}\chi_A]\frac{dT}{dt}=\Delta H_{rxn}\big|_T r_AV+\sum_{i=1}^{n}\left(-RT\frac{\nu_i}{a}\right)r_AV+\dot{Q}-\dot{W}_s \tag{20}$$

with

$$\Delta C_v=\frac{d}{a}C_{vD}+\frac{c}{a}C_{vC}-\frac{b}{a}C_{vB}-C_{vA} \tag{21}$$

or using only internal energy instead of enthalpy:

$$\sum_{i=1}^{n}[C_{vi}N_i]\frac{dT}{dt}=\Delta U_{rxn}\big|_T r_AV+\dot{Q}-\dot{W}_s \tag{22}$$

with the internal energy form of the heat of reaction given by:

$$\Delta U_{rxn}\big|_T=\Delta H_{rxn}\big|_T-\sum_{i=1}^{n}\left(RT\frac{\nu_i}{a}\right) \tag{23}$$

If the net change in the number of moles is equal to zero, then

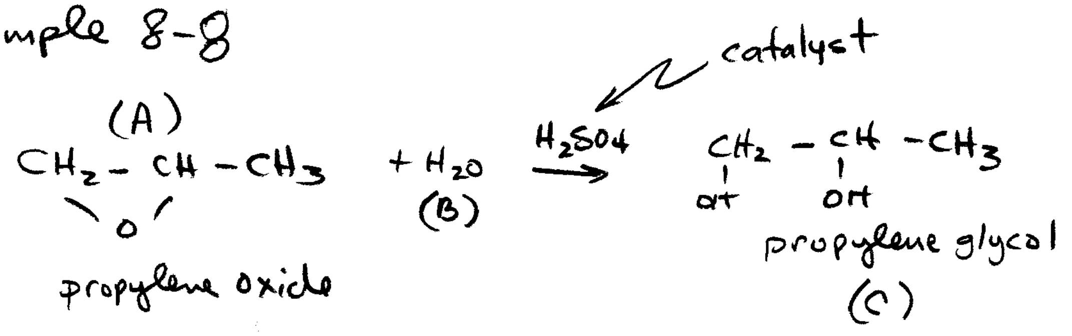
$$\Delta U_{rxn}\big|_T=\Delta H_{rxn}\big|_T \tag{24}$$

Key Point:
for a batch reactor
energy Balance there is
a difference between
a gas & liquid

Steady-state CSTR

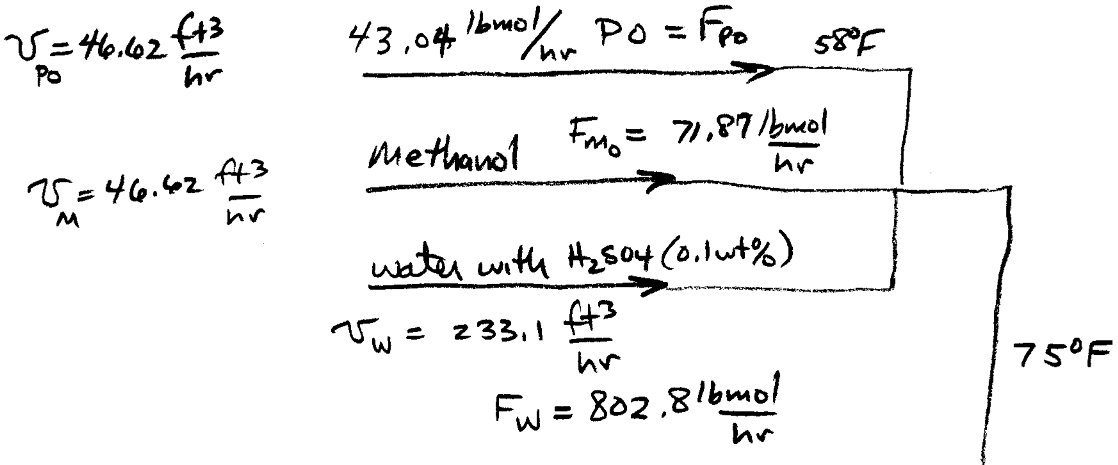
p 520

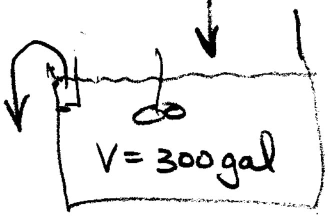
Example 8-8



Need new reactor – old one is leaking

– Overflow 300 gal reactor available (glass lined)





$k = A\exp(-E/RT)$

$T < 125°F$ (vaporization problem)

$460+125 = 585R$

can you use CSTR? – adiabatic?

ONLY V GIVEN X & T are unknown { case B page 442

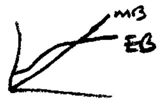
$$\left.\begin{array}{l} r_A = -kC_{PO} \\ X_{MB} = f(T) \text{ and } V \\ X_{EB} = f(T) \end{array}\right\}$$

grunt work

find H's, Cp's

Notice $\hat{C}_p$ & $\tilde{C}_p$ in eqn E8-4.6

T X_{MB} X_{EB}



T=613R which > 585R

Can't use

Example 8-8 continued

V Given ⇒ CSTR adiabatic steady-state

Mole balance

$$0 = F_0 X - k C_P V$$

C_P liquid phase $= \frac{F}{\upsilon} = \frac{F_{-}(1-X)}{\upsilon_0}$

$$0 = F_{P_0} X_P - k \frac{F_{P_0}}{\upsilon_0}(1-X)V = \boxed{X_P - k\tau(1-X_P) = 0}$$

Solve for X

$$\underbrace{\frac{\cancel{F_{P_0}} X_P}{(1-X_P)}}_{f(X)} = k \cancel{F_{P_0}} \frac{V}{\upsilon_0} = \underset{\uparrow\ A\exp(-E_A/RT)}{k}\tau$$

$f(T)$!

one equation 2 unknowns

or solving for X

$$X_P = k\tau - k\tau X_P$$

$$X_P + k\tau X_P = k\tau$$

$$\boxed{X_P = \frac{k\tau}{1+k\tau}}$$

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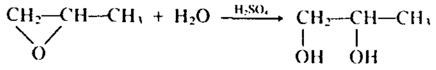
However, it is difficult to detect multiple solutions with a numerical procedure.

The algorithm for working through either Case A or B is summarized in Figure 8-3. Its application is illustrated in the following example.

Start this problem derive mole balance Ask the question What is the value of T?

Example ~~8-4~~ 8-8 Production of Propylene Glycol in an Adiabatic CSTR

Propylene glycol is produced by the hydrolysis of propylene oxide:


CH_2—CH—CH_3 + H_2O $\xrightarrow{H_2SO_4}$ CH_2—CH—CH_3 (OH)(OH)

Production, uses, and economics

Over 800 million pounds of propylene glycol were produced in 1990 and the selling price was approximately $0.56 per pound. Propylene glycol makes up about 25% of the major derivatives of propylene oxide. The reaction takes place readily at room temperature when catalyzed by sulfuric acid.

You are the engineer in charge of an adiabatic CSTR producing propylene glycol by this method. Unfortunately, the reactor is beginning to leak, and you must replace it. (You told your boss several times that sulfuric acid was corrosive and that mild steel was a poor material for construction.) There is a nice overflow CSTR of 300-gal capacity standing idle; it is glass-lined and you would like to use it.

300 gal Reactor

You are feeding 2500 lb/h (43.03 lb mol/h) of propylene oxide (P.O.) to the reactor. The feedstream consists of (1) an equivolumetric mixture of propylene oxide (46.62 ft³/h) and methanol (46.62 ft³/h), and (2) water containing 0.1 wt% H_2SO_4. The volumetric flow rate of water is 233.1 ft³/h, which is 2.5 times the methanol-P.O. flow rate. The corresponding molar feed rates of methanol and water are 71.87 and 802.8 lb mol/h, respectively. The water-propylene oxide-methanol mixture undergoes a slight decrease in volume upon mixing (approximately 3%), but you neglect this decrease in your calculations. The temperature of both feedstreams is 58°F prior to mixing, but there is an immediate 17°F temperature rise upon mixing of the two feedstreams caused by the heat of mixing. The entering temperature of all feedstreams is thus taken to be 75°F (see Figure E8-4.1).

Furosawa et al.[6] state that under conditions similar to those at which you are operating, the reaction is first-order in propylene oxide concentration and apparent zero-order in excess of water with the specific reaction rate

$$k = Ae^{-E/RT} = 16.96 \times 10^{12}(e^{-32,400/RT})\ \text{h}^{-1}$$

The units of E are Btu/lb mol.

**

There is an important constraint on your operation. Propylene oxide is a rather low-boiling substance (b.p. at 1 atm, 93.7°F). With the mixture you are using, you feel that you cannot exceed an operating temperature of 125°F, or you will lose too much oxide by vaporization through the vent system.

$T_{max} = 125°F$

Can you use the idle CSTR as a replacement for the leaking one if it will be operated adiabatically? If so, what will be the conversion of oxide to glycol?

---

[6] T. Furusawa, H. Nishimura, and T. Miyauchi, *J. Chem. Eng., Jpn.*, 2, 95 (1969).

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F_{A0} 43.03 lbmol/hr

$\varphi_A = 46.62\ \frac{ft^3}{hr}$

$\varphi_m = 46.62$

0.1% H_2SO_4 wt

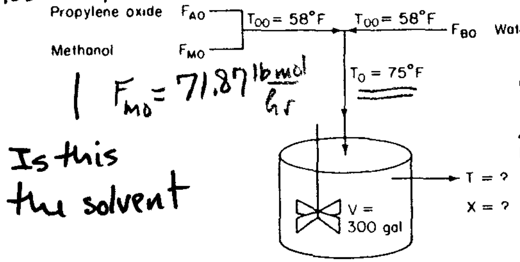


Figure E8-4.1

(H_2SO_4)

$F_{M0} = 71.87\ \frac{lbmol}{hr}$

Is this the solvent

$\varphi_B = 233.1\ \frac{ft^3}{hr}$

$F_B = 802.8\ \frac{lbmol}{hr}$

Solution

(All data used in this problem were obtained from the *Handbook of Chemistry and Physics* unless otherwise noted.) Let the reaction be represented by

$$A + B \longrightarrow C$$

in which

A is propylene oxide (MW = 58.08; ρ = 0.859 g/cm³; C_p = 35 Btu/lb mol·°F[7])
B is water (MW = 18.02; ρ = 0.9941 g/cm³; C_p = 18 Btu/lb mol·°F
C is propylene glycol (MW = 76.11; ρ = 1.036 g/cm³; C_p = 46 Btu/lb mol·°F[7])
M is methanol (MW = 32.04; ρ = 0.7914 g/cm³; C_p = 19.5 Btu/lb mol·°F)

In this problem neither the exit conversion nor the temperature of the adiabatic reactor is given. By application of the material and energy balances we can solve two equations with two unknowns (X and T). Solving these coupled equations, we determine the exit conversion and temperature for the glass-lined reactor to see if it can be used to replace the present reactor.

1. **Mole balance and design equation:**

$$F_{A0} - F_A + r_A V = 0$$

The design equation in terms of X is

$$V = \frac{F_{A0}X}{-r_A} \qquad \text{(E8-4.1)}$$

2. **Rate law:**

$$-r_A = kC_A \overset{PO}{} \qquad \text{(E8-4.2)}$$

---

[7] Estimated from the observation that the great majority of low-molecular-weight oxygen-containing organic liquids have a mass heat capacity of 0.6 cal/g·°C ± 15%.

3. **Stoichiometry** (liquid-phase, $v = v_0$):

$$C_A = C_{A0}(1 - X) \tag{E8-4.3}$$

4. **Combining** yields

$$V = \frac{F_{A0}X}{kC_{A0}(1 - X)} = \frac{v_0 X}{k(1 - X)} \tag{E8-4.4}$$

5. **Solving** for X as a function of T and recalling that $\tau = V/v_0$ gives

$$X = \frac{\tau k}{1 + \tau k} = \frac{\tau A e^{-E/RT}}{1 + \tau A e^{-E/RT}} \tag{E8-4.5}$$

This equation relates temperature and conversion through the mole balance.

6. The **energy balance** for this adiabatic reaction in which there is negligible energy input provided by the stirrer is

$$-X[\Delta H_R^\circ(T_R) + \Delta \hat{C}_p(T - T_R)] = \sum \Theta_i \tilde{C}_{pi}(T - T_0) \tag{8-41}$$

Solving for X, we obtain

$$X = \frac{\sum \Theta_i \tilde{C}_{pi}(T - T_0)}{-[\Delta H_R^\circ(T_R) + \Delta \hat{C}_p(T - T_R)]} \tag{E8-4.6}$$

This equation relates X and T through the energy balance. We see that there are two equations [equations (E8-4.5) and (E8-4.6) that must be solved for the two unknowns, X and T

7. **Calculations:**

a. Heat of reaction at temperature T:

See Perry's 6th Section 3-147

$$\Delta H_R(T) = \Delta H_R^\circ(T_R) + \Delta \hat{C}_p(T - T_R) \tag{8-27}$$

$H_A^\circ(68°\text{F})$: $-66{,}600$ Btu/lb mol[8]

$H_B^\circ(68°\text{F})$: $-123{,}000$ Btu/lb mol

$H_C^\circ(68°\text{F})$: $-226{,}000$ Btu/lb mol[8]

$$\Delta H_R^\circ(68°\text{F}) = -226{,}000 - (-123{,}000) - (-66{,}600)$$
$$= -36{,}400 \text{ Btu/lb mol propylene oxide}$$

$$\Delta \hat{C}_p = \hat{C}_{p_C} - \hat{C}_{p_B} - \hat{C}_{p_A}$$
$$= 46 - 18 - 35 = -7 \text{ Btu/lb mol}\cdot°\text{F}$$

$$\Delta H_R(T) = -36{,}400 - (7)(T - 528) \tag{E8-4.7}$$

b. Stoichiometry (C_{A0}, Θ_i, τ): The volumetric flow rate entering the reactor is

$$v_0 = v_{A0} + v_{M0} + v_{B0} \tag{E8-4.8}$$
$$= 46.62 + 46.62 + 233.1 = 326.3 \text{ ft}^3/\text{h}$$

$$V = 300 \text{ gal} = 40.1 \text{ ft}^3$$

---

[8] Calculated from heat-of-combustion data.

$$\tau = \frac{V}{v_0} = \frac{40.1 \text{ ft}^3}{326.3 \text{ ft}^3/\text{h}} = 0.1229 \text{ h} \tag{E8-4.9}$$

$$C_{A0} = \frac{F_{A0}}{v_0} = \frac{43.04 \text{ lb mol/h}}{326.3 \text{ ft}^3/\text{h}}$$
$$= 0.132 \text{ lb mol/ft}^3$$

For methanol: $\Theta_M = \frac{F_{M0}}{F_{A0}} = \frac{71.87 \text{ lb mol/h}}{43.04 \text{ lb mol/h}} = 1.67$

For water:

$$\Theta_B = \frac{F_{B0}}{F_{A0}} = \frac{802.8 \text{ lb mol/h}}{43.04 \text{ lb mol/h}} = 18.65$$

c. Energy balance terms:

$$\sum \Theta_i \tilde{C}_{pi} = \tilde{C}_{p_A} + \Theta_B \tilde{C}_{p_B} + \Theta_M \tilde{C}_{p_M} + 0C_{p_c} \tag{E8-4.10}$$
$$= 35 + (18.65)(18) + (1.67)(19.5)$$
$$= 403.3 \text{ Btu/lb mol}\cdot°\text{F}$$

$$T_0 = T_{00} + \Delta T_{\text{mix}} = 58°\text{F} + 17°\text{F} = 75°\text{F} \tag{E8-4.11}$$
$$= 535°\text{R}$$
$$T_R = 68°\text{F} = 528°\text{R}$$

The conversion calculated from the energy balance, X_{EB}, for a adiabatic reaction is found by rearranging Equation (8-41):

$$X_{EB} = -\frac{\sum \Theta_i \tilde{C}_{pi}(T - T_0)}{\Delta H_R^\circ(T_R) + \Delta \hat{C}_p(T - T_R)} \tag{E8-4.6}$$

Substituting all the known quantities into the mole and energy balances gives us

Plot X_{EB} as a function of temperature

$$X_{EB} = \frac{(403.3 \text{ Btu/lb mol}\cdot°\text{F})\ (T - 535)°\text{F}}{-[-36{,}400 - 7(T - 528)] \text{ Btu/lb mol}}$$
$$= \frac{403.3(T - 535)}{36{,}400 + 7(T - 528)} \tag{E8-4.12}$$

The conversion calculated from the mole balance, X_{MB}, is found from Equation (E8-4.5).

Plot X_{MB} as a function of temperature

$$X_{MB} = \frac{(16.96 \times 10^{12} \text{ h}^{-1})(0.1229 \text{ h}) \exp(-32{,}400/1.987T)}{1 + (16.96 \times 10^{12} \text{ h}^{-1})(0.1229 \text{ h}) \exp(-32{,}400/1.987T)}$$
$$= \frac{(2.084 \times 10^{12}) \exp(-16{,}306/T)}{1 + (2.084 \times 10^{12}) \exp(-16{,}306/T)} \tag{E8-4.13}$$

8. **Solving:** There are a number of different ways to solve these two simultaneous equations [e.g., substituting Equation (E8-4.12) into (E8-4.13)]. To give insight into the functional relationship between X and T for the mole and energy balances, we shall obtain a graphical

TABLE E8-4.1

T (°R)	X_{MB} [Eq. (E8-4.13)]	X_{EB} [Eq. (E8-4.12)]
535	0.108	0.000
550	0.217	0.166
565	0.379	0.330
575	0.500	0.440
585	0.620	0.550
595	0.723	0.656
605	0.800	0.764
615	0.860	0.872
625	0.900	0.980

solution. Here X is 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 we can learn if there is more than one intersection (i.e., multiple steady states) for which both the energy balance and mole balance are satisfied. If numerical root-finding techniques were used to solve for X and T, it would be quite possible to obtain only one root, when there is actually more than one. We shall discuss multiple steady states further in Section 8.7. We choose T and then calculate X (Table E8-4.1). The calculations are plotted in Figure E8-4.2. The virtually straight line corresponds to the energy balance [Equation (E8-4.12)] and the curved line corresponds to the mole balance [Equation (E8-4.13)]. We observe from this plot that the only intersection point is at 85% conversion and

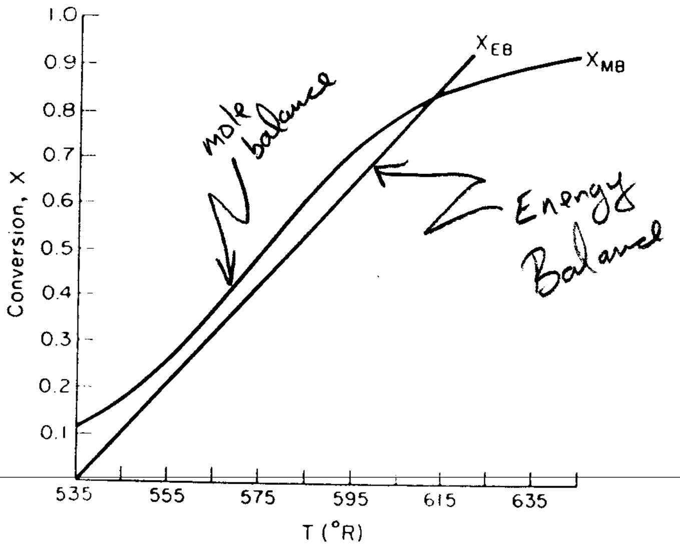


Figure E8-4.2

613°R. At this point both the energy balance and mole balance are satisfied. Because the temperature must remain below 125°F (585°R), we cannot use the 300-gal reactor as it is now.

Constant Coolant temperature

IN 3rd Edition Polymath sol'n given

$f(x) = X -$ EB

$f(T) = X -$ MB

See p. 450

Example 8-5 CSTR with a Cooling Coil

A cooling coil has been located for use in the hydration of propylene oxide discussed in Example 8-4. The cooling coil has 40 ft² of cooling surface and the cooling water flow rate inside the coil is sufficiently large that a constant coolant temperature of 85°F can be maintained. A typical overall heat-transfer coefficient for such a coil is 100 Btu/h·ft²·°F. Will the reactor satisfy the previous constraint of 125°F maximum temperature if the cooling coil is used?

Solution

If we assume that the cooling coil takes up negligible reactor volume, the conversion calculated as a function of temperature from the mole balance is the same as that in Example 8-4 [Equation (E8-4.13)].

1. **Combining the mole balance, stoichiometry,** and **rate law**, we have

As before

$$X_{MB} = \frac{2.084 \times 10^{12} \exp(-16{,}306/T)}{1 + 2.084 \times 10^{12} \exp(-16{,}306/T)} \qquad \text{(E8-4.13)}$$

2. **Energy balance:** Neglecting the work done by the stirrer, we combine equations (8-34) and (8-40) to obtain

$$\underbrace{\frac{UA(T_a - T)}{F_{A0}}}_{\text{New term}} - X[\Delta H_R^\circ(T_R) + \Delta \hat{C}_p(T - T_R)] = \sum \Theta_i \tilde{C}_{pi}(T - T_0) \qquad \text{(E8-5.1)}$$

Solving the energy balance for X_{EB} yields

$$X_{EB} = \frac{\sum \Theta_i \tilde{C}_{pi}(T - T_0) + [UA(T - T_a)/F_{A0}]}{-[\Delta H_R^\circ(T_R) + \Delta \hat{C}_p(T - T_R)]} \qquad \text{(E8-5.2)}$$

The cooling coil term in Equation (E8-5.2) is

$$\frac{UA}{F_{A0}} = 100 \frac{\text{Btu}}{\text{h·ft}^2\text{·°F}} \left(\frac{40 \text{ ft}^2}{43.04 \text{ lb mol/h}}\right) = \frac{92.9 \text{ Btu}}{\text{lb mol·°F}} \qquad \text{(E8-5.3)}$$

Recall that the cooling temperature is

$$T_a = 85°\text{F} = 545°\text{R}$$

The numerical values of all other terms of Equation (E8-5.2) are identical to those given in Equation (E8-4.12):

$$X_{EB} = \frac{403.3(T - 535) + 92.9(T - 545)}{36{,}400 + 7(T - 528)} \qquad \text{(E8-5.4)}$$

From Table E8-5.1 we see that at a temperature of 564°R, both the mole balance and energy balance are satisfied and the corresponding conversion is

TABLE E8-5.1

T	X_{MB} [Eq. (E8-4.13)]	X_{EB} [Eq. (E8-5.4)]
535	0.108	−0.025
550	0.217	0.178
→564	0.367	0.367
565	0.379	0.381
570	0.440	0.448
575	0.500	0.515
585	0.620	0.649
595	0.723	0.784

37%. Consequently, we can use the 300-gal reactor with the cooling coil successfully at a reactor temperature of 104°F. A plot of equations (E8-4.13) and (E8-5.4) will verify that there is only one steady state, at $X = 0.37$ and $T = 104°\text{F}$ (564°R).

8.3.2 Adiabatic Tubular Reactor

(See later)

The energy balance given by Equation (8-38) relates the conversion at any point in the reactor to the temperature of the reaction mixture at the same point (i.e., it gives X as a function of T). Usually, there is a negligible amount of work done on or by the reacting mixture, so normally, the work term can be neglected in tubular reactor design. However, unless the reaction is carried out adiabatically, Equation (8-38) is still difficult to evaluate, because in nonadiabatic reactors, the heat added to or removed from the system varies along the length of the reactor. This problem does not occur in adiabatic reactors, which are frequently found in industry. Therefore, the adiabatic tubular reactor will be analyzed first.

Because $\dot{Q}$ and $\dot{W}_s$ are equal to zero for the reasons stated above, Equation (8-38) reduces to

$$\boxed{X[-\Delta H_R(T)] = \int_{T_{i0}}^{T} \sum \Theta_i C_{pi}\, dT} \tag{8-43}$$

This equation can be combined with the differential mole balance

$$F_{A0}\frac{dX}{dV} = -r_A(X, T)$$

to obtain the temperature, conversion, and concentration profiles along the length of the reactor. One way of accomplishing this combination is to use Equation (8-43) to construct a table of T as a function of X. Once we have T as a function of X, we can obtain $k(T)$ as a function of X and hence $-r_A$ as a function of X alone. We then use the procedures detailed in Chapter 2 to size the different types of reactors.

Consider the elementary reversible gas-phase reaction

$$A \rightleftharpoons B$$

carried out in a PFR in which pressure drop is neglected and pure A enters the reactor.

This is an algorithm for an adiabatic PFR

Polymath on page

Design equation:

$$V = F_{A0}\int_0^X \frac{dX}{-r_A}$$

Rate law:

$$-r_A = k\left(C_A - \frac{C_B}{K_e}\right)$$

Stoichiometry ($\epsilon = 0.0$):

$$C_A = C_{A0}(1 - X)\frac{T_0}{T}$$

$$C_B = C_{A0}X\frac{T_0}{T}$$

Combining the design equation, rate law, and stoichiometry, we have

$$V = F_{A0}\int_0^X \frac{dX}{kC_{A0}[(1 - X) - (X/K_e)](T_0/T)}$$

To determine the **energy balance**, we now solve Equation (8-43) for T as a function of X and then use the equations to calculate $k(T)$ and $K_e(T)$ at a given value of X. One procedure to evaluate this integral is to

1. *Choose* $X = 0$.
2. *Calculate* T from the energy balance Equation (8-43):

$$X = \frac{\int_{T_{i0}}^{T} \sum \Theta_i C_{p_i}\, dT}{-\Delta H_R(T)}$$

For example, integrating Equation (8-43), using the mean heat capacities, and assuming $T_{i0} = T_0$, we have

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

Solving for T yields

$$T = \frac{X[-\Delta H_R^\circ(T_R)] + \sum \Theta_i \tilde{C}_{p_i} T_0 + X\,\Delta\hat{C}_p T_R}{\sum \Theta_i \tilde{C}_{p_i} + X\,\Delta\hat{C}_p}$$

3. *Calculate* T/T_0.

Example 8-8 Adiabatic CSTR

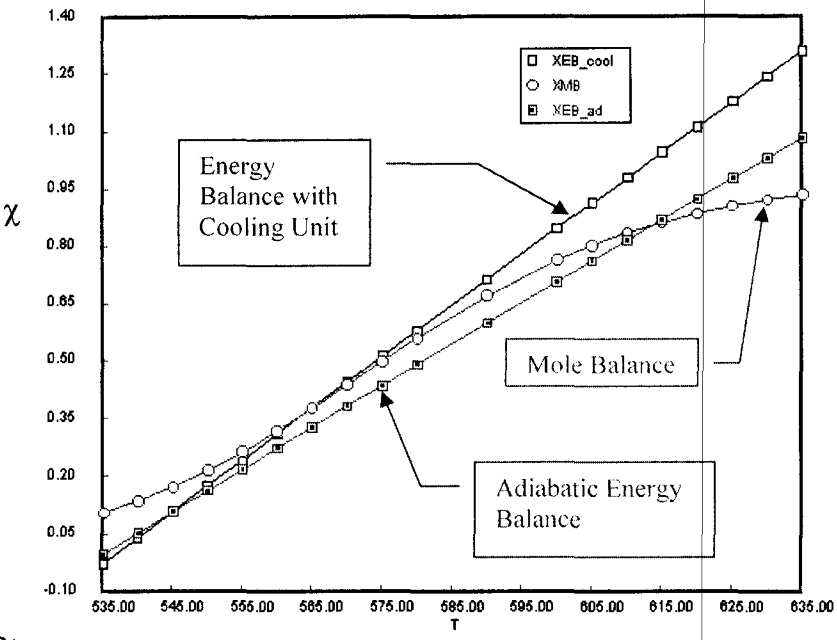
POLYMATH Report **Example 8-8 Propylene Glycol Production - Adiabatic CSTR**

Nonlinear Equations 19-Mar-2007

Calculated values of NLE variables

	Variable	Value	f(x)	Initial Guess
1	T	613.658	3.334E-09	600.
2	X	0.8573814	7.478E-11	0.8

	Variable	Value
1	A	1.696E+13
2	E	3.24E+04
3	k	48.91545
4	R	1.987
5	tau	0.1229



Nonlinear equations

1 f(X) = X-(403.3*(T-535))/(36400+7*(T-528)) = 0

2 f(T) = X-tau*k/(1+tau*k) = 0

Explicit equations

1 tau = 0.1229

2 A = 16.96*10^12

3 E = 32400

4 R = 1.987

5 k = A*exp(-E/(R*T))

Example 8-8 CSTR with Cooling Coil $\frac{UA}{F_{A0}} = 92.9\frac{\text{Btu}}{\text{lbmol°F}}$ $T_a = 545\text{ R}$

Calculated values of NLE variables

	Variable	Value	f(x)	Initial Guess
1	T	563.7289	-5.411E-10	564.
2	X	0.3636087	2.243E-11	0.367

	Variable	Value
1	A	1.696E+13
2	E	3.24E+04
3	k	4.648984
4	R	1.987
5	tau	0.1229

Nonlinear equations

1 f(X) = X-(403.3*(T-535)+92.9*(T-545))/(36400+7*(T-528)) = 0

2 f(T) = X-tau*k/(1+tau*k) = 0

Explicit equations

1 tau = 0.1229

2 A = 16.96*10^12

3 E = 32400

4 R = 1.987

5 k = A*exp(-E/(R*T))

Energy Balance Algorithm for CSTR Design – Figure 8-13, p525&526 revised

Given:
$A + B \rightarrow C$
F_{A0}, F_{B0}, r_A

Mole Balance
Energy Balance

Specifications
2 equations &
2 unknowns

Specify *X*, find *T* and *V*

Determine T
Liquids
1) Calculate *T* from energy balance
2) Calculate *k* given *T*

Gases:
1) Estimate *T* by assuming ΔH_{rxn} and C_p' are constant
2) Use Excel solver or Polymath nonlinear Equations solver (NLE) to solve for T.

Determine *V* from mole balance:

$$V = -\frac{F_{A0}\chi}{r_A}$$

Specify *V*, find *T* and *X*

A. Excel solver or POLYMATH nonlinear equation solver

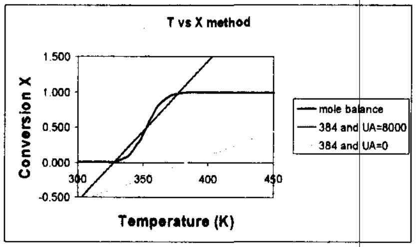
B. Graphical Solution of *X* vs *T*

$$0 = \dot{Q} - \sum_{i=1}^{n} F_{i0}\tilde{C}_{pi}(T - T_0) + \Delta H_R\big|_T (r_A V)$$

with the mass balance (below) substituted into above

$$F_{A0}\chi_A = -r_A V$$

C. Graphical solution of Q_{removed}, $Q_{\text{generated}}$ vs. *T*



Specify *T*, find *X* and *V*

Calculate *X (EB)*

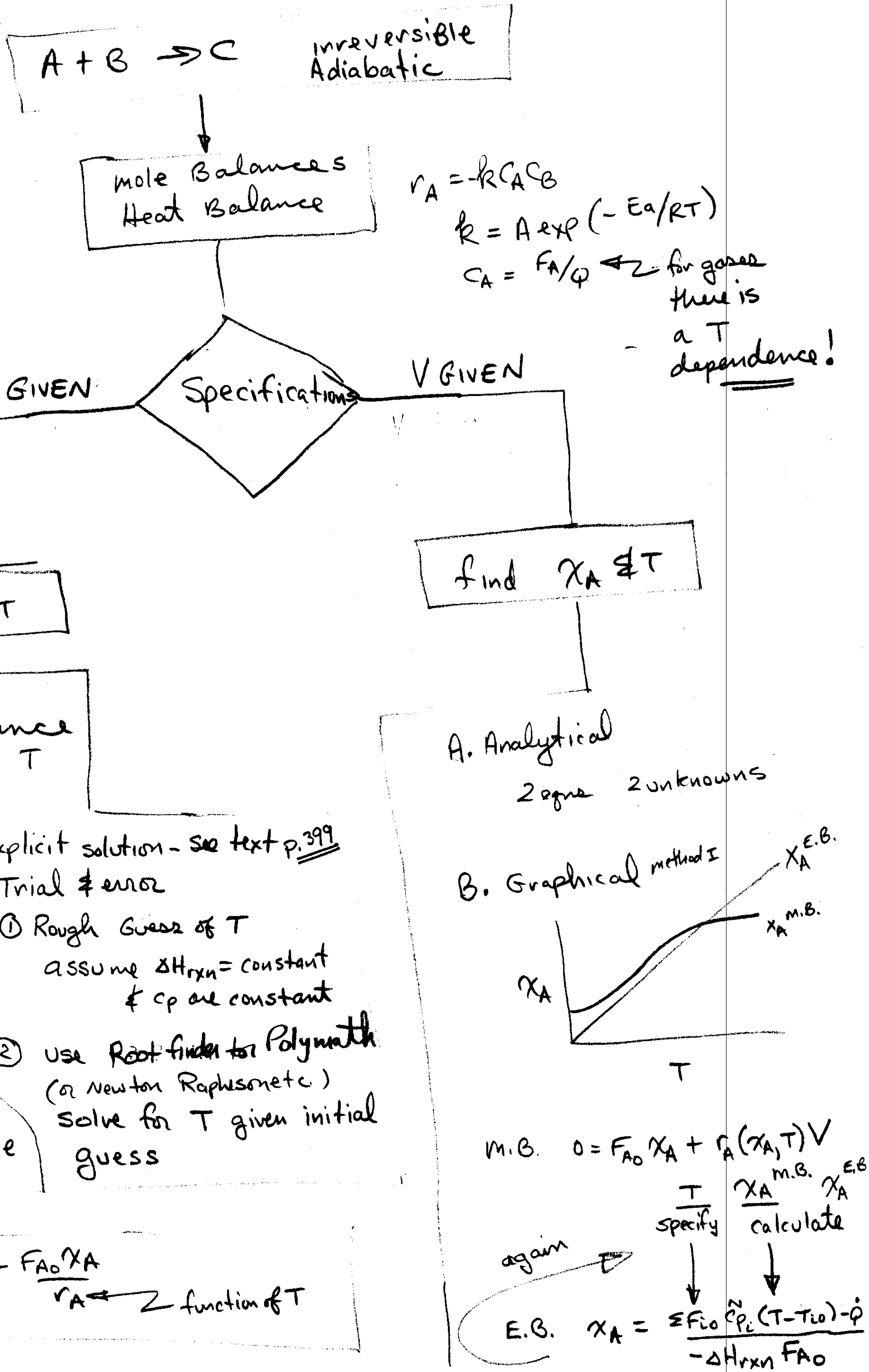
$$\Delta H_R\big|_T (F_{A0}\chi_A) = UA(T_a - T) - \dot{W}_s - \sum_{i=1}^{n} F_{i0}\tilde{C}_{pi}(T - T_0)$$

Calculate V

$$V = -\frac{F_{A0}\chi}{r_A}$$

p443 – modified

Ad



$r_A = -kC_AC_B$

$k = A\exp(-E_a/RT)$

$C_A = F_A/\varphi$ ← for gases there is a T dependence!

Note: liquids – explicit solution – see text p.399
gases – Trial & error

Ⓐ Analytical → step ① Rough Guess of T
assume ΔH_{rxn} = constant
& c_p are constant

step ② Use ~~Root finder for~~ Polymath
(or Newton Raphson etc.)
Solve for T given initial guess

Ⓑ Graphical:

$\sum F_{i0}\tilde{C}_{p_i}(T-T_{i0})-\dot{Q}$ ← line

$-\Delta H_{rxn} F_{A0} X_A$ ← curve

$$V = -\frac{F_{A0}X_A}{r_A}$$ ← function of T

A. Analytical

2 eqns 2 unknowns

B. Graphical method I

M.B. $0 = F_{A0}X_A + r_A(X_A, T)V$

T	$X_A^{M.B.}$ $X_A^{E.B}$
specify	calculate

again

E.B. $$X_A = \frac{\sum F_{i0}\tilde{C}_{p_i}(T-T_{i0})-\dot{Q}}{-\Delta H_{rxn} F_{A0}}$$

8.3.1 Steady-state CSTR

$$\frac{dT}{dt} = 0$$

$A + B \rightarrow C$ (irreversible simple reaction)

Mole Balances:

$$0 = F_{A0} - F_A + r_A V$$
$$0 = F_{B0} - F_B + \tfrac{b}{a} r_A V$$
$$0 = F_{C0} - F_C - \tfrac{c}{a} r_A V$$

$$X_A = \frac{F_{A0} - F_A}{F_{A0}}$$

$$0 = F_{A0} X_A + r_A V$$

Heat balance:

$$0 = \dot{\varphi} - \dot{w}_s - \sum_{i=1}^{n} F_{i0}\tilde{C}_{p_i}(T - T_{i0}) - \Delta H_{rxn}(-r_A V)$$

CASE 0 — Isothermal - No heat balance!

CASE I Adiabatic $\dot{\varphi} = 0$ $\dot{w}_s = 0$

CASE II NON-adiabatic

CASE I $\dot{\varphi} = 0$ $\dot{w}_s = 0$

① from mole balance: $r_A V = -(F_{A0} - F_A) = -F_{A0} X_A$

these two can be related

② $$\underbrace{\sum F_{i0} \overset{N}{C_{p_i}}(T - T_{i0})}_{\left(\frac{\text{mol } i \text{ in}}{s}\right)\frac{kJ}{\text{mol } i\, K}\, K} = -\underbrace{\Delta H_{RXN}\big|_T}_{kJ/\text{mol A React}}\, \underbrace{F_{A0}}_{\left(\frac{\text{mol A }\cancel{\text{in}}}{s}\right)} \underbrace{X_A}_{\frac{\text{mol A React}}{\cancel{\text{mol A in}}}}$$

This is a straight line for EB

unknowns: T, X_A

AND $\Delta H_{rxn} = f(T \text{ and } X_A)$

$r_A = f(T \,\&\, X_A)$

CASE II Nonadiabatic : Gaphical methods

$\underline{\underline{X_A}}$ vs T

Mole Balance : $0 = F_{A0} - F_A + r_A V = X_A F_{A0} + r_A V$ ①

Energy Balance : $0 = -\sum F_{i0} \tilde{c}_{p_i} (T - T_0) + \Delta H_{rxn} r_A V + \dot{Q} - \dot{W}_s$

Assume $\dot{W}_s = 0$

& $\dot{Q} = UA(T_a - T)$ (Heat added to C.V.) is positive $T_a > T$, is negative $T_a < T$

② $\sum F_{i0} c_{p_i} (T - T_0) - UA(T_a - T) = \Delta H_{rxn} r_A V$

Two equations : 1 & 2 (MB, EB)

unknowns : V, X_A & T } Need to specify 1 variable

if V is specified :

solve M.B. for X_A if possible (see p 399 for 1st order kinetics)

Use ~~1-2-3 Back solver~~ (Tools) Excel Solver

$0 = X_A F_{A0} + r_A V$

Procedure: Specify T calculate X_A

$k = A \exp\left(-\frac{E}{RT}\right)$

r_A is very sensitive to T

$0 < X_A \leq X_{eq} \leq 1$

excel Spread sheet

Columns

T	X_A	$f(X_A \,\&\, T)$ make = 0
100	Guess1	
110	⋮	
120	⋮	
130	⋮	

iterate on this cell

to make this cell zero

E.B. Substitute $F_{A0}X_A$ for $-r_AV$ from M.B.

$$\sum F_{i0}C_{p_i}(T-T_0) - UA(T_a-T) = -\Delta H_{rxn}F_{A0}\underset{\uparrow}{X_A}$$

only place in which X_A appears

$$X_A = \frac{+\sum F_{i0}C_{p_i}(T-T_0) - UA(T_a-T)}{-\Delta H_{rxn}F_{A0}}$$

different T's

A straight line

$$= T\left[\underbrace{\frac{(\sum F_{i0}C_{p_i}+UA)}{-\Delta H_{rxn}F_{A0}}}_{\text{Slope} = S}\right] + \left[\underbrace{\frac{-\sum F_{i0}C_{p_i}T_0 - UA\,T_a}{-\Delta H_{rxn}F_{A0}}}_{I}\right]$$

$S > 0$ $\Delta H_{rxn} < 0$ exothermic

$S < 0$ $\Delta H_{rxn} > 0$ endothermic

I: varies

spread sheet continued

T	$X_A^{M.B.}$	$f(X_A \& T)$	ΔH_{rxn}	C_p's A	B	C	$X_A^{E.B.}$ from T in column 1
100	Guess 1	make = 0	/	/	/	/	—
110			/	/	/	/	—
120			/	/	/	/	—
130							—

Straight calculation

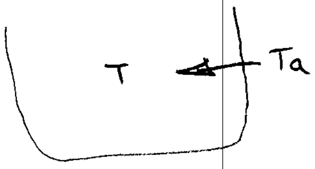
$$\boxed{\Phi_R = \Phi_G}$$

CASE II   Non-adiabatic : Graphical methods

Mole balance : $0 = F_{A0} - F_A + r_A V = X_A F_{A0} + r_A V$

Energy balance $0 = -\sum F_{i0} C_{p_i}(T - T_0) + (\Delta H_{rxn}) r_A V + \dot{\varphi} - \cancel{\dot{W}_s}^{\,0}$

$\dot{W}_s$ is it negligible? yes



$$\overbrace{\underbrace{\sum F_{i0} C_{p_i}(T - T_0) - \dot{\varphi}}_{\text{"Heat Removal"}}}^{\varphi_{R\,\text{emoved}}} = \overbrace{\underbrace{(\Delta H_{rxn}\, r_A V)}_{\text{"Heat generated"}}}^{\Phi_{\text{Generated}}}$$

"Heat Removal" $\xrightarrow{\text{exo}}$ "Heat generated"

"added" $\xrightarrow{\text{endo}}$ "Heat required"

if $\dot{\varphi} = U A_{HT}(T_a - T)$ if $T_a > T$ heat is added; $T_a < T$ heat is removed

(positive is adding heat to the system)

Looking at the Φ_{Removed} term $\Phi_R = \sum F_{i0} C_{p_i}(T - T_0) - UA(T_a - T)$

$$= \underbrace{(\sum F_i C_{p_i} + UA)}_{\text{Slope}} T \underbrace{- \overbrace{\sum F_{i0} C_{p_i} T_0}^{} - UA\, T_a}_{\text{intercept}}$$

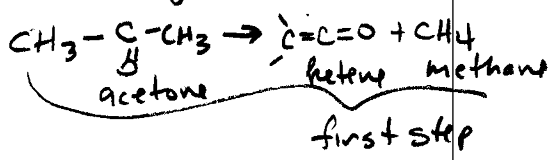
This analysis is useful for stability

504 4th Ed ENERGY Balance PFR

8-5 Table E8-7.1

Example 8-7
Production of Acetic Anhydride

$A \rightarrow B + C$



$$\underbrace{\underset{\text{acetone}}{CH_3-\overset{}{\underset{O}{C}}-CH_3} \rightarrow \underset{\text{ketene}}{CH_2=C=O} + \underset{\text{methane}}{CH_4}}_{\text{first step}}$$

$$\frac{dF_A}{dV} = r_A \qquad \frac{dF_B}{dV} = -r_A \qquad F_C = F_B$$

$$r_A = -kC_A$$

$$k = \exp\left[34.34 - \frac{34{,}222\,K}{T}\right]$$

$$F_T = F_A + F_B + F_C$$

$$\frac{dT}{dV} = \frac{Ua\,(T_a - T) + r_A\,\Delta H_{A\,rxn}}{F_A C_{P_A} + F_B C_{P_B} + F_C C_{P_C}}$$

my equation 13 in PFR (from hand out) and Foglers eqn 8-60

$\Delta H_{rxn}\big|_{T_R} = 80{,}770$ J/mol ← Watch Units

$$C_A = F_A / Q$$

$$Q = \frac{Q_0 \cancel{P_0} F_T T}{\cancel{P} F_{T0} T_0} \qquad \text{assuming } P = P_0$$

$\left.\begin{matrix} C_{P_A} \\ C_{P_B} \\ C_{P_C} \end{matrix}\right\}$ Ideal Gas heat capacities $\quad a + bT + cT^3 \; [=] \; \frac{J}{mol\,K}$

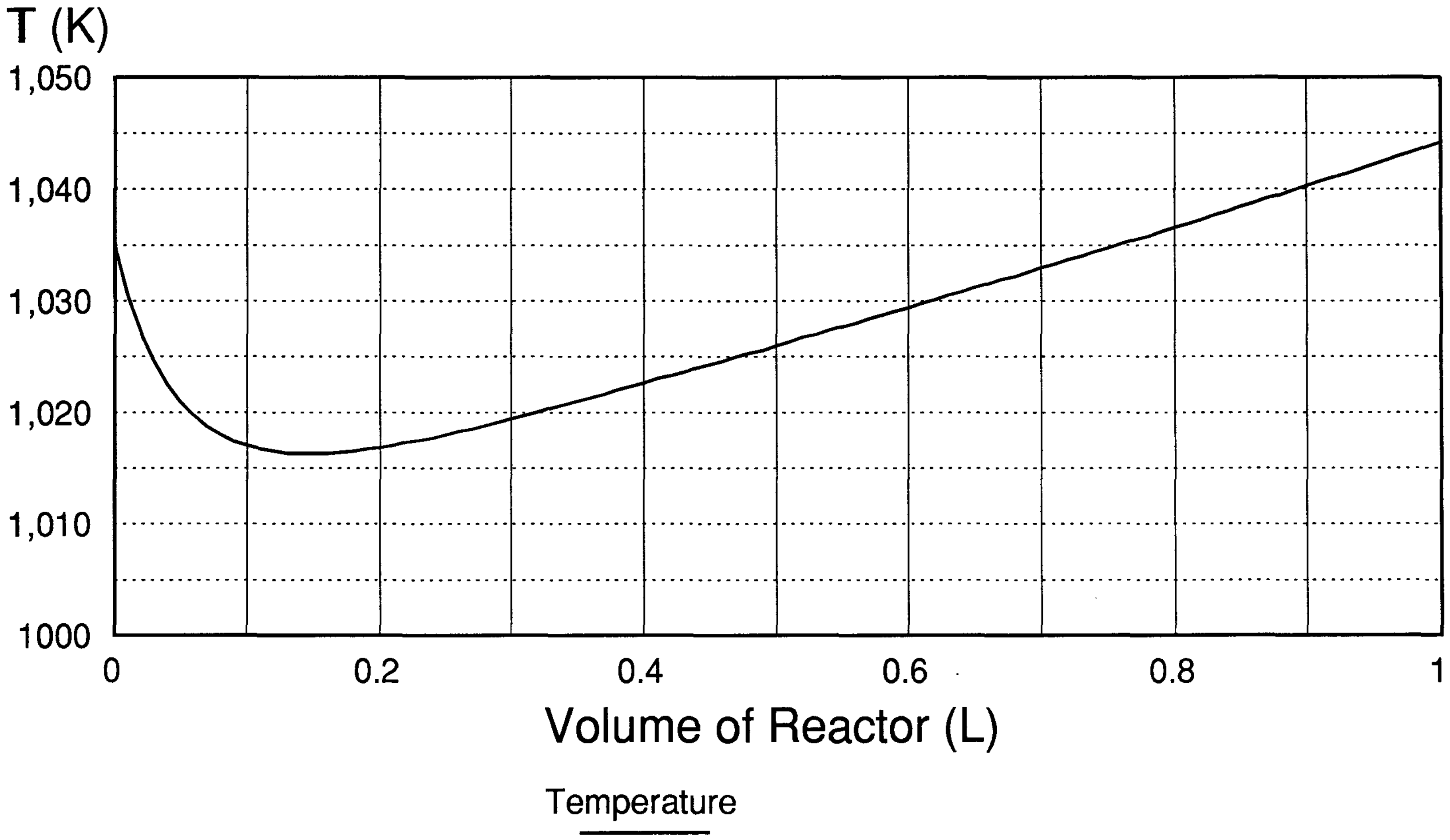
$$\Delta H_{Rxn}\big|_T = \Delta H_{rxn}\big|_{T_R} + \Delta C_p\,(T - T_R)$$

$$\Delta\hat{C}_p = C_{P_C} + C_{P_B} - C_{P_A}$$

Concentration and Temperature Profiles

Heated Plug Flow Reactor with Endothermic Rxn

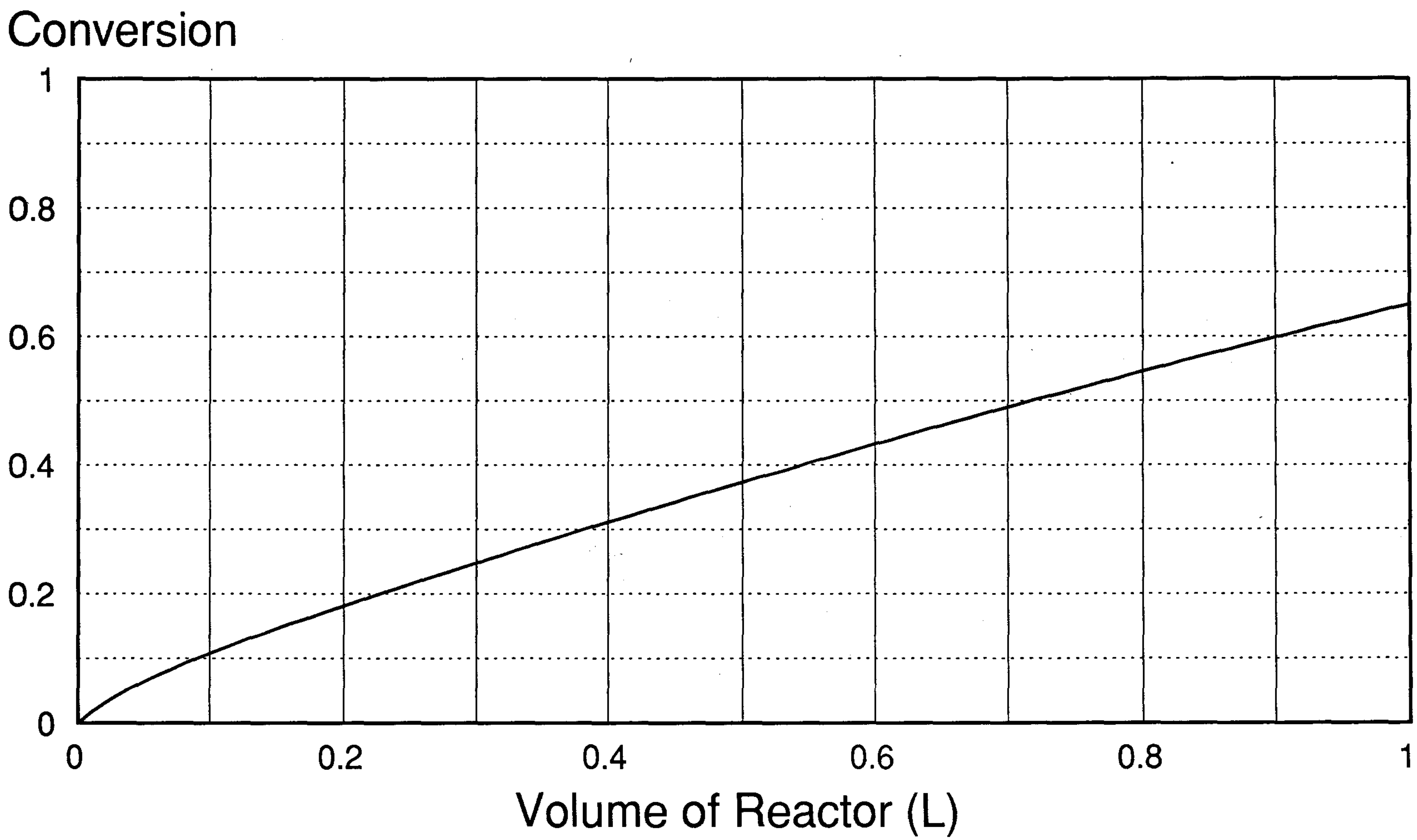
Example Problem 8-7 (Fogler 1991)



Concentration and Temperature Profiles

Heated Plug Flow Reactor with Endothermic Rxn

Example Problem 8-7 (Fogler 1991)



POLYMATH 5.0 Results

Example 8-7 03-22-2000

Calculated values of the DEQ variables

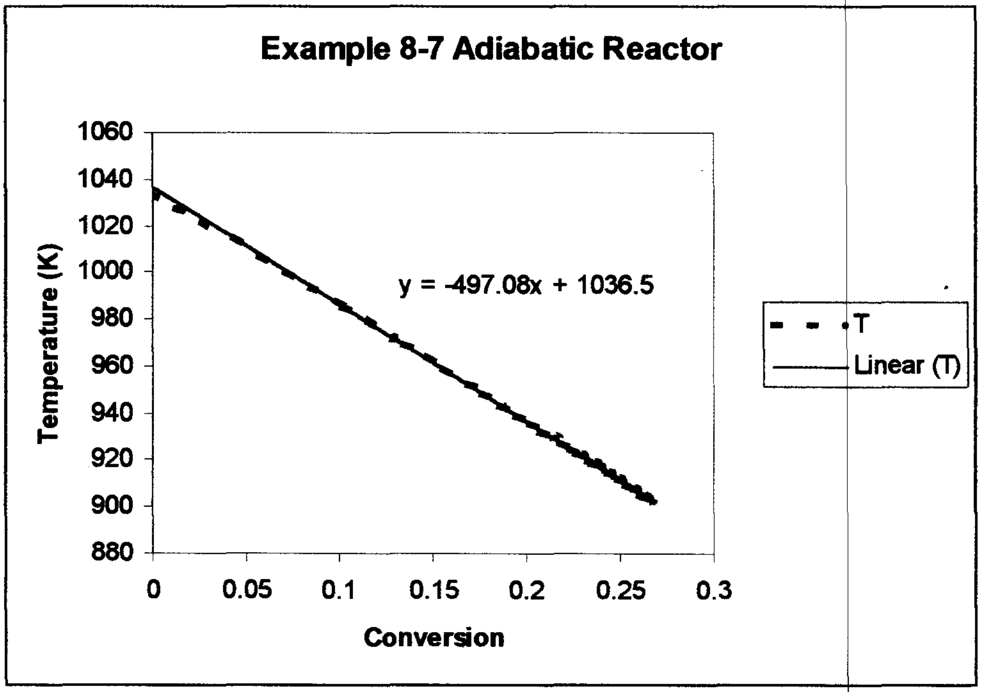
```
Variable  initial value  minimal value  maximal value  final value
V          0              0              5              5
X          0              0              0.2684425      0.2684425
T          1035           902.59769      1035           902.59769
Fao        38.3           38.3           38.3           38.3
Cpa        166.90862      154.44403      166.90862      154.44403
delCp     -9.1838673     -9.1838673     -6.6838142     -6.6838142
k          3.5808176      0.0280243      3.5808176      0.0280243
Cao        18.8           18.8           18.8           18.8
To         1035           1035           1035           1035
Tr         298            298            298            298
deltaH     7.876E+04      7.876E+04      7.981E+04      7.981E+04
ra        -67.319371     -67.319371     -0.3484305     -0.3484305
```

ODE Report (RKF45)

Differential equations as entered by the user
[1] d(X)/d(V) = -ra/Fao
[2] d(T)/d(V) = -ra*(-deltaH)/(Fao*Cpa+X*delCp)

Explicit equations as entered by the user
[1] Fao = 38.3
[2] Cpa = 26.63+.183*T-45.86*10^(-6)*T^2
[3] delCp = 6.8-11.5*10^(-3)*T-3.81*10^(-6)*T^2
[4] k = 8.2*10^14*exp(-34222/T)
[5] Cao = 18.8
[6] To = 1035
[7] Tr = 298
[8] deltaH = 80770+6.8*(T-Tr)-5.75*10^(-3)*(T^2-Tr^2)-1.27*10^(-6)*(T^3-Tr^3)
[9] ra = -k*Cao*(1-X)/(1+X)*To/T

Independent variable
variable name : V
initial value : 0
final value : 5



POLYMATH 5.0 Results

Example 8-7 Part B 03-22-2000

Calculated values of the DEQ variables

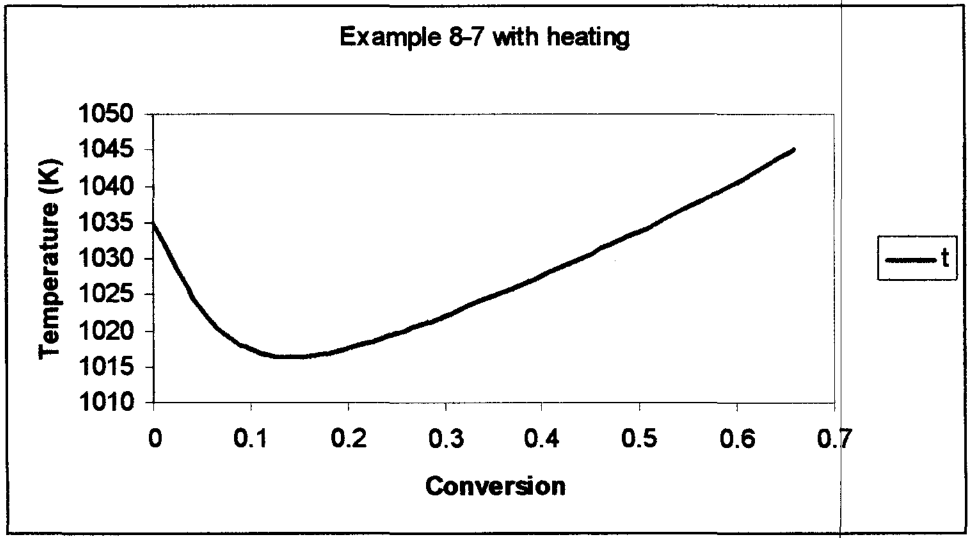
```
Variable  initial value  minimal value  maximal value  final value
v          0              0              0.001          0.001
x          0              0              0.6590103      0.6590103
t          1035           1016.253       1045.0786      1045.0786
fa0        0.0376         0.0376         0.0376         0.0376
ua         1.65E+04       1.65E+04       1.65E+04       1.65E+04
ta         1150           1150           1150           1150
cpa        166.83577      165.17143      167.7179       167.7179
dcp       -9.1838673     -9.3796454     -8.8220385     -9.3796454
ca0        18.8           18.8           18.8           18.8
t0         1035           1035           1035           1035
term      -1374.4629     -1415.9993     -1299.3832     -1415.9993
dh         7.876E+04      7.866E+04      7.893E+04      7.866E+04
ra        -67.304        -67.304        -18.845559     -18.845559
```

ODE Report (RKF45)

```
Differential equations as entered by the user
 [1]  d(x)/d(v) = -ra/fa0
 [2]  d(t)/d(v) = (ua*(ta-t)+ra*dh)/(fa0*(cpa+x*dcp))

Explicit equations as entered by the user
 [1]  fa0 = .0376
 [2]  ua = 16500
 [3]  ta = 1150
 [4]  cpa = 26.6+.183*t-.0000459*t*t
 [5]  dcp = 6.8-.0115*t-.00000381*t*t
 [6]  ca0 = 18.8
 [7]  t0 = 1035
 [8]  term = -.00000127*(t^3-298^3)
 [9]  dh = 80770+6.8*(t-298)-.00575*(t^2-298^2)+term
 [10]  ra = -ca0*3.58*exp(34222*(1/t0-1/t))*(1-x)*(t0/t)/(1+x)

Independent variable
 variable name : v
 initial value : 0
 final value : 0.001
```



Notes on Plug Flow Reactors

See page 477 -478 Table 8-1

A) Ideal Exam problem $A \rightarrow B + C$

Adiabatic $\dot{q} = 0$

pure feed → $\Sigma F_{i0} C_{p_i} = F_{A0} C_{pA}$

$\Delta H_{rxn} \simeq$ constant

$\therefore \Delta \hat{C}_p \simeq 0$

$\Delta C_p \simeq 0$

$$\frac{dT}{dV} = \frac{\Delta H_{rxn}|_T \, r_A}{F_{A0} C_{pA}}$$

B) Hand Calculations to check Polymath or Aspen

① assume: $\Delta H_{rxn} =$ constant or use an average value

② $r_A|_{max} = k C_{A0}$ ← feed temperature

③ $C_p =$ constant (this will vary with T)

$$\frac{\Delta T}{\Delta V} = \frac{\Delta H_{rxn}(-k C_{A0})}{\Sigma F_i C_{p_i}}$$ — put in numbers

C) Units

$$\frac{dT}{dV} = \frac{\Delta H_{rxn}|_T \, r_A + \dot{q}}{\Sigma F_i C_{p_i}} \qquad \frac{dT}{dW} = \frac{\Delta H_{rxn} r_A' + \dot{q}}{\Sigma F_i C_{p_i}}$$

if $\dot{q} = Ua(T_a - T)$

← a must have a change in units

$U [=] \frac{J}{s \, m_{sa}^2 K}$ $T [=] K$

$a [=] \frac{m_{sa}^2}{m^3_{Reactor}}$

$\dot{q} [=] \frac{J}{s \, m_{sa}^2 \cancel{K}} \frac{m_{sa}^2}{m_R^3} \cancel{K} = \frac{J}{s \, m_R^3}$

$\dot{q}$ – must be $\frac{J}{s \, kg_{cat}}$

$a = ?$

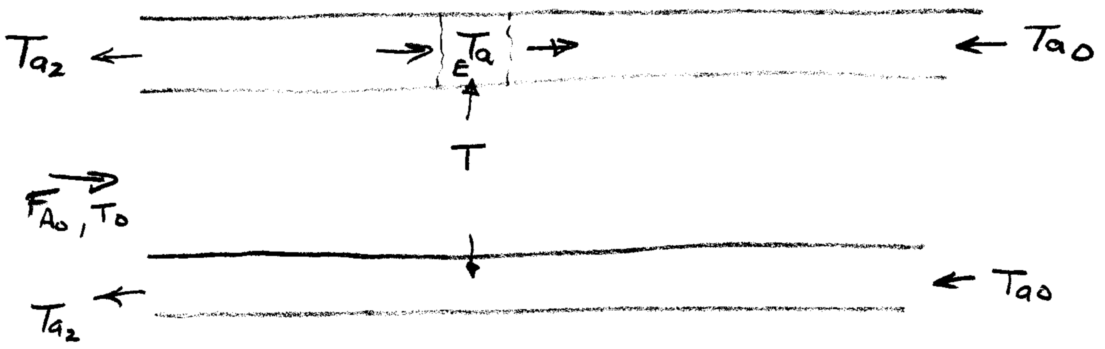
$$\underset{U}{\frac{J}{s \, m_{sa}^2 K}} \; \underset{a}{\frac{m_{sa}^2}{m_R^3}} \; \underset{\frac{1}{(1-\phi)}}{\frac{m_R^3}{m_{cat}^3}} \; \underset{\frac{1}{\rho_c}}{\frac{m_{cat}^3}{kg_{cat}}} \; \underset{(T_a - T)}{K} = \dot{q}$$

Section 8.4.2

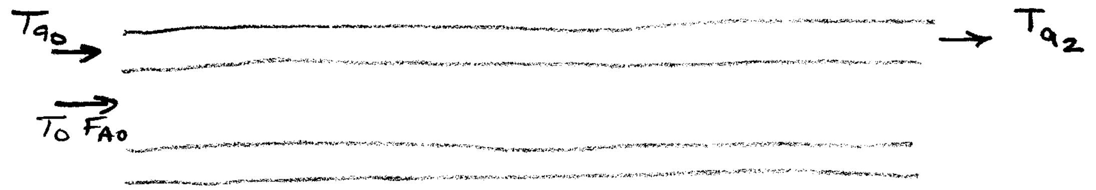
Co-current vs Counter Current

Energy balance on cooling or heat exchanger fluid

Counter current



Co current



Energy balance on cooling fluid (Co-current)

$$\underbrace{\frac{V_{exchanger}}{V_{Reactor}}\Delta V \cancel{\frac{\partial E}{\partial t}}}_{0} = \dot{m}_c C_p T_a\big|_V - \dot{m}_c C_p T_a\big|_{V+\Delta V} + U a \Delta V (T - T_a)$$

$$\frac{kg}{s}\ \frac{J}{\cancel{kg}\ \cancel{°C}}\ \cancel{°C} \qquad \frac{J}{m^2\ \cancel{°C}\ s}\ \frac{m^2}{m^3}\ \cancel{°C}$$

$$\frac{J}{s}$$

$$\lim \Delta V \to 0 \quad \frac{V_{exch}}{V_{react}} \frac{\partial E}{\partial t} = -\dot{m} \frac{\partial C_p T_a}{\partial V} + U a (T - T_a)$$

at S.S.

$$\dot{m}_c \frac{\partial C_p T_a}{\partial V} = U a (T - T_a) \qquad \text{Co-current } 8\text{-}40$$

$$\dot{m}_c \frac{\partial (C_p T_a)}{\partial V} = -U a (T - T_a) \qquad \text{Counter current } 8\text{-}41$$

Plug flow Reactors

$$\frac{dT}{dV} = \frac{\Delta H_{rxn}\big|_T r_A + \dot{q}}{\sum F_{i0} C_{p_i} + \Delta C_p F_{A0} X_A}$$

① If $\Delta C_p \rightarrow$ small or $X_A \rightarrow$ small then $\Delta H_{rxn} \sim$ constant

mole balance
$$-F_{A0}\frac{dX_A}{dV} = r_A$$

② $\dot{q} = 0$

$$\frac{dT}{dV} = \frac{\Delta H_{rxn}}{\sum F_{i0} C_{p_i}} r_A = \frac{\Delta H_{rxn}}{\sum F_{i0} C_{p_i}}\left(\frac{dF_A}{dV}\right) = \frac{\Delta H_{rxn}}{\sum F_{i0} C_{p_i}}(F_{A0})\left(\frac{-dX_A}{dV}\right)$$

$$\int_{T_0}^{T} dT = -\frac{\Delta H_{rxn}}{\sum F_{i0} C_{p_i}} F_{A0} \int_{0}^{X_A} dX_A$$

$$\frac{\sum F_{i0} \tilde{C}_{p_i}}{-\Delta H_{rxn}} \frac{(T - T_0)}{F_{A0}} = X_A \quad \leftarrow \text{for PFR}$$

$$X_A = \frac{\sum (F_{i0}/F_{A0}) \tilde{C}_{p_i} (T - T_0)}{-\Delta H_{rxn}\big|_T} \quad \leftarrow \text{CSTR}$$

These are the same!

Θ_i in Book!

Predicting Equilibrium Constants

see appendix C p ~~878~~ 2nd
929 3rd
1021 4th

$$K_a \equiv \exp\left(-\frac{\Delta G^\circ_{Rxn}}{RT}\right)$$

$$aA + bB \rightleftharpoons rR + sS$$

$$K_a = \prod_{i=1} a_i^{\nu_i} = \frac{a_R^r \, a_S^s}{a_A^a \, a_B^b}$$

ν_i – (stoichiometric coefficient)
−a, −b, r and s

$$\left\{ \begin{aligned} a_i &\equiv \frac{f_i}{f_i^o} = \gamma_i y_i P \\ &= \gamma_i x_i P_i^{vap} \end{aligned} \right.$$

liquid

for an ideal gas $a_i = y_i P$ or P_i

$$\therefore \quad K_a = K_p = \frac{P_R^r \, P_S^s}{P_A^a \, P_B^b} = \exp\left(-\frac{\Delta G_{rxn}}{RT}\right)$$

The equilibrium constant K_C

$$K_C \equiv \frac{C_R^r \, C_S^s}{C_A^a \, C_B^b}$$

Converting to pressure $C_i = \frac{N_i}{V} = \frac{P_i}{RT}$

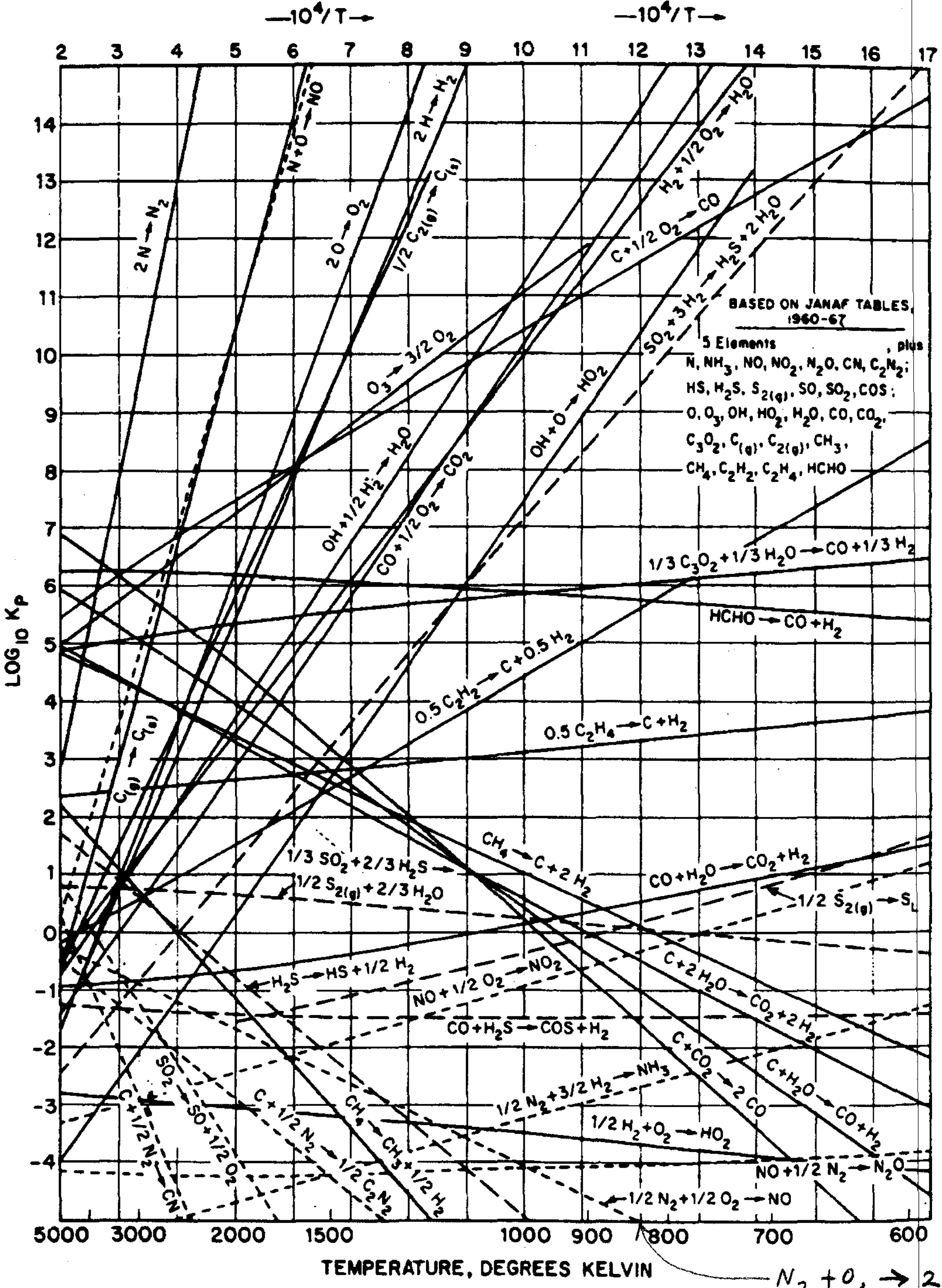
$$K_C = \frac{(P_R/RT)^r \, (P_S/RT)^s}{(P_A/RT)^a \, (P_B/RT)^b} = \frac{P_r^r \, P_S^s}{P_A^a \, P_B^b} \left(\frac{1}{RT}\right)^{r+s-a-b}$$

$$\therefore \quad K_C = K_P \left(\frac{1}{RT}\right)^{r+s-a-b}$$

From Figure EC-1.1 we read at 1000 K that log K_P = 0.15; therefore, K_P = 1.41, which is close to the calculated value. We note that there is no net change in the number of moles for this reaction; therefore,

$$K = K_p = K_c \text{ (dimensionless)}$$

Taking the square root of Equation (EC-1.7) yields



$N_2 + O_2 \rightarrow 2NO$

Figure EC-1.1 From M. Modell and R. Reid, *Thermodynamics and Its Applications*, © 1983. Reprinted by permission of Prentice Hall, Inc., Upper Saddle River, N.J.

The van't Hoff equation can be used to adjust the equilibrium constant for temperature

a function of T

$$\frac{d \ln K_p}{dT} = \frac{\Delta H_{rxn}}{RT^2}$$

If ΔH_{rxn} is assumed to be constant over small ranges of temperature

$$\ln K_p \Big|_{K_{p_1}}^{K_{p_2}} = -\left(\frac{\Delta H_{rxn}}{RT}\right)\Big|_{T_1}^{T_2}$$

$$\ln(K_{p_2}/K_{p_1}) = -\frac{\Delta H_{rxn}}{R}\left(\frac{1}{T_2} - \frac{1}{T_1}\right)$$

Example - simple cases

Note for complex (Real) mixtures you need a computer code!

$$K_a \equiv \exp\left(-\frac{\Delta G_{rxn}}{RT}\right)$$

$G = H - TS$

$$N_2 + O_2 \rightleftharpoons 2NO$$

CRC 57th D-73

CRC 74th p5-3

$\Delta G^\circ_{N_2}\Big|_{25°C} = 0$

CRC57th D-74

$\Delta G^\circ_{O_2}\Big|_{25°C} = 0$

$\Delta G^\circ_{NO}\Big|_{25°C} = 20.719 \frac{kcal}{mol}$

20.72 D-73 CRC 57th

at

$$\Delta G^\circ_{rxn}\Big|_{25°C} = 2\Delta G^\circ_{NO} - \Delta G^\circ_{O_2} - \Delta G^\circ_{O_2}$$

$$= 2\left(20.719 \frac{kcal}{mol}\right) - 0 - 0$$

$$= 41.44\ kcal/mol$$

$$K_p = \exp\left(-\frac{41.44\ kcal/mol \left(\frac{10^3 cal}{1 kcal}\right)}{\left(1.987 \frac{cal}{mol\ K}\right)(273+25)}\right)$$

$$= 4.04 \times 10^{-30} \text{ at } 25°C$$

Exists as all O_2 and N_2

Example Problem: Find K_p at 25°C

$$N_2 + O_2 \rightleftharpoons 2NO$$

$\Delta G^{o}_{N_2}\big|_{25°C} = 0$

CRC 57th D-73 & 74

CRC 74th p 5-3

$\Delta G^{o}_{O_2}\big|_{25°C} = 0$

$\Delta G^{o}_{NO}\big|_{25°C} = 20.72$ kcal/mol

$$\Delta G^{o}_{rxn} = 2\Delta G^{o}_{NO} - \Delta G^{o}_{N_2} - \Delta G^{o}_{O_2} = 2(20.72)\ \mathrm{kcal/mol}$$

$$= 41.44\ \mathrm{kcal/mol}$$

$$K_p = \exp\left[- \frac{41.44\ \mathrm{kcal/mol}\left(\frac{10^3\ \mathrm{cal}}{\mathrm{kcal}}\right)}{\left(\frac{1.987\ \mathrm{cal}}{\mathrm{mol\ K}}\right)(273+25)\mathrm{K}} \right]$$

$$= 4.04 \times 10^{-30} \text{ at } 25°C$$

exists as all O_2 & N_2 at 25°C

CRC 74th 5-67 for NO

Find K_p at 2700K

$$\Delta H^{o}_{rxn} = 2H^{o}_{f\,NO} - H^{o}_{f\,O_2} - H^{o}_{f\,N_2}$$

$$= 2\left(21.60\ \frac{\mathrm{kcal}}{\mathrm{mol}}\right) - 0 - 0$$

$$= 43.2\ \mathrm{kcal/mol}$$

Endothermic

Does ΔH_{rxn} change with T?

Sandler, ChE Thermo

$$\hat{C}_p = \int_{T_1}^{T_2} c_p \, dT = a\Delta T + \frac{b}{2}\left(T_2^2 - T_1^2\right) + \frac{c}{3}\left(T_2^3 - T_1^3\right) + \frac{d}{4}\left(T_2^4 - T_1^4\right)$$

	a	$b \times 10^2$	$c \times 10^5$	$d \times 10^9$
NO	6.461	0.2358	−0.07705	0.08729
O_2	6.732	0.1505	−0.01791	0
N_2	6.529	0.1488	−0.02271	0

Eq 8-25

$$\Delta C_{p_{rxn}} = 2\hat{C}_{p_{NO}} - \hat{C}_{p_{O_2}} - C_{p_{N_2}}$$

$$\int_{298}^{2700k} \Delta C_{p_{rxn}} dT \quad 2(20{,}120) - 20416 - 19552 = 273 \text{ cal/mol}$$

$$\Delta H_{rxn}\Big|_T = \Delta H^\circ_{rxn}\Big|_{298k} + \int_{298}^{2700} \Delta C_p \, dT$$ Eqn 8-26 p. 434

$$\Delta H_{rxn} = 43{,}200 \text{ cal/mol} + \underbrace{273 \text{ cal/mol}}_{\text{this is small} \;\therefore\; \Delta H_{rxn} \overset{\sim}{=} \text{const.}}$$

$$\ln\left(\frac{K_{p_2}}{K_{p_1}}\right) = -\frac{\left(\overset{\text{(average)}}{43{,}200} + \frac{273}{2}\right)}{1.987 \frac{\text{cal}}{\text{mol K}}}\left[\frac{1}{2700} - \frac{1}{298}\right]$$

$$K_{p_2} = 0.076$$

ON PDF

Find favorable reactions faster

Equations for Gibbs free energy will help identify favorable reactions

C. L. Yaws and **P-Y. Chiang,** Lamar University, Beaumont, Texas

A RECENT ARTICLE[1] reported equations to help calculate the heat of reaction for proposed organic chemical reactions. In that article, enthalpy equations were given for 700 major organic compounds.

Now, equations are given to identify whether the reactions are thermodynamically favorable. The method uses Gibbs free energy of formation for the reactants and products. The equation for any 700 major organic compounds is given as temperature coefficients. Then the reaction can be tested at various temperature levels beyond the standard 298°K conditions imposed by many other data tabulations. Data for water and hydrogen chloride are also included.

Gibbs free energy of formation of ideal gas (ΔG_f, kjoule/g-mol) is calculated from the tabulated coefficients (A, B, C) and the temperature (T, °K) using the following equation:

$$\Delta G_f = A + BT + CT^2 \qquad (1)$$

Chemical equilibrium for a reaction is associated with the change in Gibbs free energy (ΔG_r) calculated as follows:

$$\Delta G_r = \Delta G_{f,\,products} - \Delta G_{f,\,reactants} \qquad (2)$$

If the change in Gibbs free energy is negative, the thermodynamics for the reaction are favorable. On the other hand, if the change in Gibbs free energy is highly positive, the thermodynamics for the reaction are not favorable and may be feasible only under special circumstances. Rough criteria for screening chemical reactions are as follows:

$\Delta G_r < 0$ kjoules/g-mol	favorable
$0 < \Delta G_r < 50$ kjoules/g-mol	possibly favorable
$\Delta G_r > 50$ kjoules/g-mol	not favorable

Example. Calculate the change in Gibbs free energy for the reaction of methanol and oxygen to produce formaldehyde and water at reaction temperatures of 600, 700, 800, 900 and 1,000°K:

$$CH_4O(g) + 0.5\ O_2(g) \rightarrow CH_2O(g) + H_2O(g)$$

Using correlation constants from Table 1 (see pp. 82–84) and Eq. 1 at temperature of 600°K, we obtain:

$$\begin{aligned} \Delta G_{f,CH_2O} &= -115.972 + 1.663*10^{-2}(600) \\ &\quad + 1.138*10^{-5}(600^2) = -101.9 \\ \Delta G_{f,H_2O} &= -241.74 + 4.174*10^{-2}(600) \\ &= +7.428*10^{-6}(600^2) = -214.02 \\ \Delta G_{f,CH_4O} &= -201.860 + 1.254*10^{-1}(600) \\ &= +2.035*10^{-5}(600^2) = -119.28 \\ \Delta G_{f,O_2} &= 0 \end{aligned}$$

The change in Gibbs free energy for the reaction is determined from Eq. 2 and the Gibbs free energy of formation for the products and reactants:

$$\begin{aligned} \Delta G_r &= \Delta G_{f,CH_2O} + \Delta G_{f,H_2O} - \Delta G_{f,CH_4O} - 0.5*\Delta G_{f,O_2} \\ &= -101.9 + (-214.02) - (-119.28) - 0 \\ &= -196.64 \text{ kjoule/g-mol} \end{aligned}$$

Repeating the calculations at the other temperatures gives these results:

T, °K	600	700	800	900	1.000
G_r, kJ/g-mol	−197	−204	−210	−217	−224

Since the change in Gibbs free energy for the reaction is highly negative, the thermodynamics for the reaction at these temperatures are favorable (reaction promising).

Data source. The correlation constants were determined from a least-squares fit of data from the literature.[2-13] In most cases, average deviations between calculated and reported data were less than 0.6 kjoules/g-mol.

A copy (5¼ inch floppy disk) of a menu-driven computer program to calculate Gibbs free energy of formation and change in Gibbs free energy for reactions (including random access data file of compound coefficients) is available for a nominal fee. For details, contact: C. L. Yaws, Dept. of Chem. Engg., Lamar University, P.O. Box 10053, Beaumont, Texas 77710, USA.

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The authors

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TABLE 1—Gibbs free energy of formation of gas, $\Delta G_f = A + BT + CT^2$

NO.	FORMULA	NAME	A	B	C	DEL GF @298K
1	CCL4	CARBON-TETRACHLORIDE	-100.838	1.4561E-01	-8.6766E-06	-58.24
2	CCL3F	TRICHLOROFLUOROMETHANE	-284.764	1.3487E-01	-5.3707E-06	-245.18
3	CCL2F2	DICHLORODIFLUOROMETHANE	-481.826	1.4482E-01	4.3398E-06	-438.36
4	CCLF3	CHLOROTRIFLUOROMETHANE	-694.327	1.3545E-01	6.8525E-07	-653.96
5	CF4	CARBON-TETRAFLUORIDE	-933.816	1.5206E-01	6.7334E-08	-888.43
6	CO	CARBON-MONOXIDE	-109.885	-9.2218E-02	1.4547E-06	-137.25
7	CO2	CARBON-DIOXIDE	-393.360	-3.8212E-03	1.3322E-06	-394.38
8	COS	CARBONYL-SULFIDE	-136.376	-1.0575E-01	2.5162E-05	-165.64
9	CS2	CARBON-DISULFIDE	121.242	-1.9750E-01	5.0587E-05	66.90
10	CHCL3	CHLOROFORM	-101.846	1.1137E-01	8.6302E-07	-68.53
11	CHCL2F	DICHLOROFLUOROMETHANE	-283.827	1.0295E-01	3.0690E-06	-252.31
12	CHCLF2	CHLORODIFLUOROMETHANE	-482.201	1.0493E-01	4.2461E-06	-450.47
13	CHF3	TRIFLUOROMETHANE	-698.169	1.1528E-01	7.1054E-06	-663.38
14	CHI3	TRIIODOMETHANE	116.349	1.0932E-01	-2.3734E-06	177.95
15	CHNS	ISOTHIOCYANIC-ACID	129.895	-6.6463E-02	3.1215E-05	112.88
16	CH2CL2	DICHLOROMETHANE	-95.965	8.8080E-02	8.5438E-06	-68.87
17	CH2CLF	CHLOROFLUOROMETHANE	-262.549	8.3336E-02	1.0838E-05	-236.54
18	CH2F2	DIFLUOROMETHANE	-453.610	9.0621E-02	1.2721E-05	-425.35
19	CH2I2	DIIODOMETHANE	53.345	9.2134E-02	3.1467E-06	101.09
20	CH2O	FORMALDEHYDE	-115.972	1.6630E-02	1.1381E-05	-109.91
21	CH2O2	FORMIC-ACID	-379.192	9.1431E-02	9.5249E-06	-351.00
22	CH3BR	BROMOMETHANE	-55.241	8.0199E-02	1.1207E-05	-28.16
23	CH3CL	CHLOROMETHANE	-86.903	7.5722E-02	1.4823E-05	-62.89
24	CH3F	FLUOROMETHANE	-234.475	7.6613E-02	1.6807E-05	-209.99
25	CH3I	IODOMETHANE	-20.627	8.3254E-02	8.0701E-06	15.65
26	CH3NO2	NITROMETHANE	-76.173	2.2736E-01	1.4355E-05	-6.95
27	CH3NO2	METHYL-NITRITE	-65.640	2.2023E-01	9.2945E-06	1.00
28	CH3NO3	METHYL-NITRATE	-122.358	3.0626E-01	8.2197E-06	-30.17
29	CH4	METHANE	-75.262	7.5925E-02	1.8700E-05	-50.84
30	CH4O	METHANOL	-201.860	1.2542E-01	2.0345E-05	-162.51
31	CH4S	METHANETHIOL	-19.483	1.6198E-02	5.2738E-05	-9.92
32	CH5N	METHYLAMINE	-24.115	1.8179E-01	2.2182E-05	32.26
33	C2CL4	TETRACHLOROETHENE	-12.176	1.1919E-01	-7.6720E-06	22.64
34	C2CL6	HEXACHLOROETHANE	-142.168	2.9199E-01	-1.8349E-05	-56.82
35	C2CL3F3	112TRICHLOROTRIFLUOROETHANE	-696.127	2.7082E-01	-1.6970E-05	-617.14
36	C2CL2F4	12DICHLOROTETRAFLUOROETHANE	-888.420	2.8167E-01	-1.2046E-05	-805.42
37	C2CLF5	CHLOROPENTAFLUOROETHANE	-1108.395	2.8235E-01	-6.2604E-06	-1025.08
38	C2F4	TETRAFLUOROETHENE	-658.653	1.1776E-01	-1.8295E-06	-623.71
39	C2F6	HEXAFLUOROETHANE	-1344.410	2.9411E-01	-7.6769E-06	-1257.38
40	C2N2	CYANOGEN	309.375	-3.9443E-02	-4.0226E-06	297.19
41	C2HCL3	TRICHLOROETHENE	-9.886	8.7331E-02	-1.0392E-06	16.07
42	C2HCL5	PENTACHLOROETHANE	-143.234	2.5953E-01	-9.0227E-06	-66.65
43	C2HF3	TRIFLUOROETHENE	-491.035	8.7927E-02	3.6243E-06	-464.47
44	C2H2	ACETYLENE(ETHYNE)	227.187	-6.1675E-02	4.3960E-06	209.20
45	C2H2CL2	1,1-DICHLOROETHENE	1.994	7.6745E-02	5.2089E-06	25.40
46	C2H2CL2	CIS-1,2-DICHLOROETHENE	-3.264	7.5010E-02	5.9732E-06	19.66
47	C2H2CL2	TRANS-1,2-DICHLOROETHENE	-0.772	7.4474E-02	5.8258E-06	22.01
48	C2H2CL4	1,1,2,2-TETRACHLOROETHANE	-153.859	2.2902E-01	-5.6905E-07	-85.56
49	C2H2F2	1,1-DIFLUOROETHENE	-337.271	7.8515E-02	7.9741E-06	-313.09
50	C2H2F2	CIS-1,2-DIFLUOROETHENE	-322.591	7.4587E-02	9.0983E-06	-299.49
51	C2H2F2	TRANS-1,2-DIFLUOROETHENE	-322.543	7.5116E-02	8.3671E-06	-299.32
52	C2H2O	KETENE	-60.986	2.0204E-04	6.7660E-06	-60.29
53	C2H3BR	BROMOETHYLENE	61.115	5.6200E-02	8.8699E-06	80.75
54	C2H3CL	CHLOROETHENE	31.557	3.2864E-02	1.8788E-05	42.93
55	C2H3CL3	1,1,2-TRICHLOROETHANE	-139.616	2.0630E-01	5.9155E-06	-77.49
56	C2H3CLO	ACETYL-CHLORIDE	-244.471	1.2418E-01	1.2494E-05	-206.23
57	C2H3F	FLUOROETHENE	-139.376	4.3674E-02	1.3376E-05	-125.06
58	C2H3F3	1,1,1-TRIFLUOROETHANE	-746.790	2.2467E-01	9.9950E-06	-678.77
59	C2H3N	ACETONITRILE	87.546	5.6339E-02	1.3233E-05	105.60
60	C2H4	ETHYLENE	51.752	4.9338E-02	1.7284E-05	68.12
61	C2H4BR2	1,2-DIBROMOETHANE	-72.860	1.9515E-01	3.5902E-06	-10.59
62	C2H4CL2	1,1-DICHLOROETHANE	-131.060	1.9006E-01	1.2939E-05	-73.09
63	C2H4CL2	1,2-DICHLOROETHANE	-130.549	1.8562E-01	1.3775E-05	-73.85
64	C2H4F2	1,1-DIFLUOROETHANE	-494.858	1.9101E-01	1.6948E-05	-436.22
65	C2H4I2	1,2-DIIODOETHANE	0.000	1.9267E-01	5.9773E-06	78.49
66	C2H4O	ETHYLENE-OXIDE	-53.838	1.3048E-01	1.8741E-05	-13.10
67	C2H4O	ACETALDEHYDE	-167.052	1.0714E-01	1.8665E-05	-133.30
68	C2H4O2	ACETIC-ACID	-435.963	1.9346E-01	1.6362E-05	-376.69
69	C2H4O2	METHYL-FORMATE	-350.914	1.7474E-01	1.6322E-05	-297.19
70	C2H4OS	THIOACETIC-ACID	-178.876	6.9466E-02	4.6167E-05	-154.01
71	C2H4S	THIACYCLOPROPANE	85.451	2.2403E-02	5.2946E-05	96.90
72	C2H5BR	BROMOETHANE	-83.274	1.7808E-01	1.4544E-05	-26.32
73	C2H5CL	CHLOROETHANE	-112.949	1.7104E-01	1.9992E-05	-60.00
74	C2H5F	FLUOROETHANE	-262.745	1.7117E-01	2.2082E-05	-209.53
75	C2H5I	IODOETHANE	-45.122	1.8148E-01	1.1291E-05	21.34
76	C2H5N	ETHYLENIMINE	121.662	1.8205E-01	2.0521E-05	177.99
77	C2H5NO2	NITROETHANE	-103.424	3.2377E-01	1.9797E-05	-4.90
78	C2H5NO3	ETHYL-NITRATE	-156.474	3.9637E-01	1.3852E-05	-36.86
79	C2H6	ETHANE	-85.787	1.6858E-01	2.6853E-05	-32.93
80	C2H6O	METHYL-ETHER	-185.257	2.3378E-01	2.7075E-05	-112.93
81	C2H6O	ETHYL-ALCOHOL	-236.102	2.1904E-01	2.3659E-05	-168.28
82	C2H6O2	ETHYLENE-GLYCOL	-390.502	2.8378E-01	1.4492E-05	-304.47
83	C2H6S	METHYL-SULFIDE	-33.596	1.1704E-01	6.2933E-05	6.95
84	C2H6S	ETHANETHIOL	-42.415	1.0784E-01	6.1979E-05	-4.69
85	C2H6S2	METHYL-DISULFIDE	-18.556	8.6388E-02	8.3731E-05	14.73
86	C2H7N	ETHYLAMINE	-47.732	2.7622E-01	2.6932E-05	37.28
87	C2H7N	DIMETHYLAMINE	-20.837	2.8875E-01	2.7736E-05	67.99
88	C3H3N	ACRYLONITRILE	184.585	3.2496E-02	1.0680E-05	195.31
89	C3H4	ALLENE(PROPADIENE)	191.839	3.0752E-02	1.4194E-05	202.38
90	C3H4	PROPYNE(METHYLACETYLENE)	185.351	2.5730E-02	1.6771E-05	194.43
91	C3H4O2	ACRYLIC-ACID	-337.271	1.6672E-01	1.5209E-05	-286.06
92	C3H5BR	3-BROMO-1-PROPENE	30.623	1.5305E-01	1.3603E-05	79.96
93	C3H5CL	3-CHLORO-1-PROPENE	-1.565	1.4516E-01	1.9444E-05	43.60
94	C3H5CL3	1,2,3-TRICHLOROPROPANE	-187.124	2.9501E-01	1.3833E-05	-97.78
95	C3H5I	3-IODO-1-PROPENE	60.299	1.6149E-01	8.7329E-06	120.16
96	C3H5N	PROPIONITRILE	49.759	1.4902E-01	2.0199E-05	96.15
97	C3H6	PROPENE	19.412	1.3685E-01	2.5749E-05	62.72
98	C3H6	CYCLOPROPANE	51.643	1.6873E-01	2.4956E-05	104.39
99	C3H6BR2	1,2-DIBROMOPROPANE	-108.362	2.8677E-01	1.0766E-05	-17.66
100	C3H6CL2	1,2-DICHLOROPROPANE	-167.410	2.7636E-01	1.9161E-05	-83.09
101	C3H6CL2	1,3-DICHLOROPROPANE	-162.984	2.6293E-01	2.0036E-05	-82.59
102	C3H6CL2	2,2-DICHLOROPROPANE	-177.370	3.0654E-01	1.3973E-05	-84.56
103	C3H6I2	1,2-DIIODOPROPANE	-33.335	2.8806E-01	7.3960E-06	76.52
104	C3H6O	PROPYLENE-OXIDE	-94.384	2.2200E-01	2.4413E-05	-25.77
105	C3H6O	ALLYL-ALCOHOL	-133.300	2.0021E-01	2.4167E-05	-71.25
106	C3H6O	PROPIONALDEHYDE	-193.326	2.0318E-01	2.3446E-05	-130.46
107	C3H6O	ACETONE	-218.777	2.1177E-01	2.6619E-05	-153.05
108	C3H6S	THIACYCLOBUTANE	64.908	1.2220E-01	6.8322E-05	107.49
109	C3H7BR	1-BROMOPROPANE	-108.651	2.7327E-01	1.9373E-05	-22.47
110	C3H7BR	2-BROMOPROPANE	-117.884	2.8906E-01	1.7035E-05	-27.24
111	C3H7CL	1-CHLOROPROPANE	-131.804	2.6332E-01	2.6786E-05	-50.67
112	C3H7CL	2-CHLOROPROPANE	-148.229	2.7943E-01	2.4248E-05	-62.51
113	C3H7F	1-FLUOROPROPANE	-282.862	2.6769E-01	2.8109E-05	-200.29
114	C3H7F	2-FLUOROPROPANE	-290.498	2.8041E-01	2.7211E-05	-204.22
115	C3H7I	1-IODOPROPANE	-69.399	2.8216E-01	1.4073E-05	27.95
116	C3H7I	2-IODOPROPANE	-80.618	2.9402E-01	1.3004E-05	20.08
117	C3H7NO2	1-NITROPROPANE	-127.329	4.1957E-01	2.5482E-05	0.33
118	C3H7NO2	2-NITROPROPANE	-142.923	4.2813E-01	2.4433E-05	-12.80
119	C3H7NO3	PROPYL-NITRATE	-177.035	4.9531E-01	1.9599E-05	-27.32
120	C3H7NO3	ISOPROPYL-NITRATE	-194.076	5.0799E-01	1.8793E-05	-40.67
121	C3H8	PROPANE	-105.603	2.6475E-01	3.2500E-05	-23.47
122	C3H8O	ETHYL-METHYL-ETHER	-218.142	3.2628E-01	3.2734E-05	-117.65
123	C3H8O	PROPYL-ALCOHOL	-259.317	3.1232E-01	3.3063E-05	-162.97
124	C3H8O	ISOPROPYL-ALCOHOL	-274.608	3.2915E-01	2.9243E-05	-173.59
125	C3H8S	ETHYL-METHYL-SULFIDE	-55.315	2.0160E-01	7.3615E-05	11.42
126	C3H8S	1-PROPANETHIOL	-63.596	1.9853E-01	7.3301E-05	2.18
127	C3H8S	2-PROPANETHIOL	-72.286	2.1257E-01	7.0456E-05	-2.55
128	C3H9N	PROPYLAMINE	-74.693	3.7313E-01	3.2876E-05	39.79
129	C3H9N	TRIMETHYLAMINE	-26.507	4.0989E-01	3.2215E-05	98.91
130	C4F8	OCTAFLUOROCYCLOBUTANE	-1530.065	4.4414E-01	-1.3877E-05	-1398.84
131	C4H2	BUTADIYNE(BIACETYLENE)	473.689	-9.9298E-02	-6.6000E-07	443.96
132	C4H4	1BUTEN3YNE(VINYLACETYLENE)	304.509	1.1570E-03	1.1754E-05	305.98
133	C4H4O	FURAN	-35.958	1.1791E-01	1.7007E-05	0.88
134	C4H4S	THIOPHENE	118.623	1.2478E-02	4.9100E-05	126.78
135	C4H6	1,2-BUTADIENE	161.456	1.1686E-01	2.2211E-05	198.45
136	C4H6	1,3-BUTADIENE	109.172	1.3296E-01	1.9003E-05	150.67
137	C4H6	1-BUTYNE(ETHYLACETYLENE)	164.525	1.1892E-01	2.1726E-05	202.09
138	C4H6	2-BUTYNE(DIMETHYLACETYLENE)	145.727	1.2497E-01	2.5536E-05	185.43
139	C4H6	CYCLOBUTENE	128.171	1.4815E-01	2.4315E-05	174.72
140	C4H6O3	ACETIC-ANHYDRIDE	-578.076	3.3162E-01	2.5188E-05	-476.68
141	C4H7N	BUTYRONITRILE	32.613	2.4673E-01	2.5125E-05	108.66
142	C4H7N	ISOBUTYRONITRILE	23.812	2.5960E-01	2.4170E-05	103.60
143	C4H8	1-BUTENE	-1.692	2.3442E-01	3.1582E-05	71.30
144	C4H8	2-BUTENE,CIS	-8.619	2.3793E-01	3.6144E-05	65.86
145	C4H8	2-BUTENE,TRANS	-12.497	2.4252E-01	3.2484E-05	62.97
146	C4H8	2-METHYLPROPENE	-18.295	2.4609E-01	3.0860E-05	58.07
147	C4H8	CYCLOBUTANE	24.216	2.7677E-01	3.3570E-05	110.04
148	C4H8BR2	1,2-DIBROMOBUTANE	-135.879	3.9161E-01	1.6038E-05	-13.14
149	C4H8BR2	2,3-DIBROMOBUTANE	-139.240	4.0686E-01	1.5194E-05	-11.92
150	C4H8I2	1,2-DIIODOBUTANE	-58.978	3.9654E-01	1.1910E-05	82.09
151	C4H8O	BUTYRALDEHYDE	-206.702	2.9866E-01	2.9382E-05	-114.77
152	C4H8O	2-BUTANONE	-239.887	3.0451E-01	3.0949E-05	-146.06
153	C4H8O2	P-DIOXANE	-318.550	4.5161E-01	3.0870E-05	-180.79
154	C4H8O2	ETHYL-ACETATE	-444.960	3.8444E-01	2.9614E-05	-327.40
155	C4H8S	THIACYCLOPENTANE	-29.540	2.2963E-01	7.8684E-05	46.02
156	C4H9BR	1-BROMOBUTANE	-129.464	3.7268E-01	2.3816E-05	-12.89
157	C4H9BR	2-BROMOBUTANE	-142.489	3.7386E-01	2.1226E-05	-25.77
158	C4H9BR	2-BROMO-2-METHYLPROPANE	-155.863	4.1286E-01	1.6443E-05	-28.16
159	C4H9CL	1-CHLOROBUTANE	-149.464	3.6039E-01	3.2740E-05	-38.79
160	C4H9CL	2-CHLOROBUTANE	-163.844	3.5979E-01	3.1321E-05	-53.47
161	C4H9CL	1-CHLORO-2-METHYLPROPANE	-161.758	3.6555E-01	3.1330E-05	-49.66
162	C4H9CL	2-CHLORO-2-METHYLPROPANE	-185.492	3.9793E-01	2.7814E-05	-64.10
163	C4H9I	2-IODO-2-METHYLPROPANE	-113.912	4.1708E-01	1.1495E-05	23.64
164	C4H9N	PYRROLIDINE	-6.977	3.9482E-01	3.9541E-05	114.68
165	C4H9NO2	1-NITROBUTANE	-147.096	5.1673E-01	3.1532E-05	10.13
166	C4H9NO2	2-NITROBUTANE	-166.954	5.2869E-01	3.0809E-05	-6.23
167	C4H10	BUTANE	-128.375	3.6047E-01	3.8256E-05	-17.15
168	C4H10	2-METHYLPROPANE(ISOBUTANE)	-136.800	3.7641E-01	3.7497E-05	-20.88
169	C4H10O	ETHYL-ETHER	-254.382	4.3005E-01	3.8901E-05	-122.34
170	C4H10O	METHYL-PROPYL-ETHER	-239.994	4.2359E-01	3.8666E-05	-109.91
171	C4H10O	METHYL-ISOPROPYL-ETHER	-254.443	4.3538E-01	3.8072E-05	-120.88
172	C4H10O	BUTYL-ALCOHOL	-276.720	4.0989E-01	3.9100E-05	-150.67
173	C4H10O	SEC-BUTYL-ALCOHOL	-294.630	4.1501E-01	3.6367E-05	-167.32
174	C4H10O	TERT-BUTYL-ALCOHOL	-328.304	4.4891E-01	3.4426E-05	-191.04
175	C4H10S	ETHYLSULFIDE	-78.870	2.9895E-01	8.3578E-05	17.78
176	C4H10S	ISOPROPYL-METHYL-SULFIDE	-85.853	3.0788E-01	8.3375E-05	13.43
177	C4H10S	METHYL-PROPYL-SULFIDE	-77.076	2.9483E-01	8.4110E-05	18.41
178	C4H10S	1-BUTANETHIOL	-83.578	2.9249E-01	8.2267E-05	11.05
179	C4H10S	2-BUTANETHIOL	-91.727	3.0122E-01	8.1363E-05	5.40
180	C4H10S	2-METHYL-1-PROPANETHIOL	-92.734	3.0510E-01	8.1489E-05	5.56
181	C4H10S	2-METHYL-2-PROPANETHIOL	-105.410	3.3262E-01	7.7086E-05	0.71
182	C4H10S2	ETHYL-DISULFIDE	-68.636	2.7360E-01	1.0136E-04	22.26
183	C4H11N	BUTYLAMINE	-94.792	4.7000E-01	3.9129E-05	49.20
184	C4H11N	SEC-BUTYLAMINE	-107.194	4.8307E-01	3.8180E-05	40.63
185	C4H11N	TERT-BUTYLAMINE	-123.074	4.9817E-01	3.4076E-05	28.87
186	C4H11N	DIETHYLAMINE	-75.362	4.8136E-01	3.9617E-05	72.09
187	C5H5N	PYRIDINE	138.330	1.6730E-01	2.0124E-05	190.20
188	C5H6S	2-METHYLTHIOPHENE	87.227	1.0101E-01	6.1872E-05	122.93
189	C5H6S	3-METHYLTHIOPHENE	86.422	9.9868E-02	6.2512E-05	121.84
190	C5H8	1,2-PENTADIENE	144.351	2.1311E-01	2.5804E-05	210.41
191	C5H8	1,3-PENTADIENE,CIS	76.492	2.2279E-01	2.9198E-05	145.77
192	C5H8	1,3-PENTADIENE,TRANS	76.388	2.2756E-01	2.5564E-05	146.73
193	C5H8	1,4-PENTADIENE	104.148	2.1318E-01	2.5915E-05	170.25
194	C5H8	2,3-PENTADIENE	137.273	2.2032E-01	3.0252E-05	205.89
195	C5H8	3-METHYL-1,2-BUTADIENE	128.505	2.2625E-01	2.7245E-05	198.61
196	C5H8	2-METHYL-1,3-BUTADIENE	74.305	2.3206E-01	2.4048E-05	145.85
197	C5H8	1-PENTYNE	143.273	2.1581E-01	2.7158E-05	210.25
198	C5H8	2-PENTYNE	127.758	2.1215E-01	3.2628E-05	194.18
199	C5H8	3-METHYL-1-BUTYNE	135.083	2.2757E-01	2.6485E-05	205.32
200	C5H8	CYCLOPENTENE	30.597	2.5615E-01	3.8896E-05	110.79
201	C5H8	SPIROPENTANE	182.924	2.6664E-01	2.9124E-05	265.31
202	C5H10	1-PENTENE	-22.938	3.3006E-01	3.7449E-05	79.12
203	C5H10	2-PENTENE,CIS	-30.293	3.2915E-01	4.0930E-05	71.84
204	C5H10	2-PENTENE,TRANS	-33.667	3.3463E-01	3.9095E-05	69.91
205	C5H10	2-METHYL-1-BUTENE	-38.406	3.3676E-01	3.6799E-05	65.61
206	C5H10	3-METHYL-1-BUTENE	-30.771	3.4337E-01	3.2419E-05	74.77
207	C5H10	2-METHYL-2-BUTENE	-44.552	3.3614E-01	4.0962E-05	59.66
208	C5H10	CYCLOPENTANE	-80.495	3.8452E-01	4.5171E-05	38.62
209	C5H10BR2	2,3-DIBROMO-2-METHYLBUTANE	-177.701	5.2964E-01	1.6349E-05	-13.35
210	C5H10O	VALERALDEHYDE	-229.987	3.9652E-01	3.5518E-05	-108.28
211	C5H10O	2-PENTANONE	-260.842	4.0269E-01	3.7677E-05	-137.07
212	C5H10S	THIACYCLOHEXANE	-59.519	3.5205E-01	8.4273E-05	53.05
213	C5H10S	CYCLOPENTANETHIOL	-43.019	3.0720E-01	9.3808E-05	57.03
214	C5H11BR	1-BROMOPENTANE	-152.750	4.7242E-01	2.7996E-05	-5.73
215	C5H11CL	1-CHLOROPENTANE	-177.625	4.5745E-01	3.8765E-05	-37.40
216	C5H11CL	1-CHLORO-3-METHYLBUTANE	-183.095	4.5557E-01	3.6144E-05	-43.68
217	C5H11CL	2-CHLORO-2-METHYLBUTANE	-205.548	4.8810E-01	3.5442E-05	-56.48
218	C5H12	PENTANE	-149.141	4.5748E-01	4.4617E-05	-8.37
219	C5H12	2-METHYLBUTANE(ISOPENTANE)	-157.445	4.6399E-01	4.3411E-05	-14.81
220	C5H12	2,2-DIMETHYPROPANE	-169.088	5.0284E-01	3.9605E-05	-15.23
221	C5H12O	METHYL-TERT-BUTYL-ETHER	-296.013	5.5806E-01	4.2094E-05	-125.44
222	C5H12O	PENTYL-ALCOHOL	-305.155	5.0637E-01	4.5232E-05	-149.75
223	C5H12O	TERT-PENTYL-ALCOHOL	-332.312	5.4443E-01	4.2371E-05	-165.77
224	C5H12S	BUTYL-METHYL-SULFIDE	-97.062	3.8661E-01	9.3888E-05	26.65
225	C5H12S	ETHYL-PROPYL-SULFIDE	-99.575	3.8453E-01	9.4240E-05	23.56
226	C5H12S	2-METHYL-2-BUTANETHIOL	-122.516	4.1515E-01	8.8234E-05	9.20
227	C5H12S	1-PENTANETHIOL	-103.448	3.8392E-01	9.2649E-05	19.37
228	C6CL6	HEXACHLOROBENZENE	-34.385	2.6934E-01	-1.8686E-05	44.18
229	C6F6	HEXAFLUOROBENZENE	-957.239	2.6465E-01	-1.1629E-05	-879.39
230	C6H4CL2	O-DICHLOROBENZENE	28.788	1.7721E-01	1.0481E-05	82.68
231	C6H4CL2	M-DICHLOROBENZENE	25.238	1.7541E-01	1.0191E-05	78.58
232	C6H4CL2	P-DICHLOROBENZENE	21.845	1.8209E-01	1.0115E-05	77.15

NO.	FORMULA	NAME	A	B	C	DEL GF @298K
233	C6H4F2	M-DIFLUOROBENZENE	-311.294	1.7786E-01	1.2420E-05	-257.02
234	C6H4F2	O-DIFLUOROBENZENE	-295.933	1.7694E-01	1.1637E-05	-242.00
235	C6H4F2	P-DIFLUOROBENZENE	-308.558	1.8283E-01	1.2013E-05	-252.84
236	C6H5BR	BROMOBENZENE	85.584	1.6480E-01	1.3600E-05	138.53
237	C6H5CL	CHLOROBENZENE	50.479	1.5737E-01	1.7618E-05	99.16
238	C6H5F	FLUOROBENZENE	-118.073	1.5842E-01	1.8022E-05	-69.04
239	C6H5I	IODOBENZENE	125.947	1.6680E-01	9.7930E-06	187.78
240	C6H6	BENZENE	81.512	1.5282E-01	2.6522E-05	129.66
241	C6H6O	PHENOL	-97.896	2.1140E-01	1.9980E-05	-32.89
242	C6H6S	BENZENETHIOL	114.974	9.1284E-02	6.0204E-05	147.61
243	C6H7N	2-PICOLINE	96.687	2.6032E-01	2.7720E-05	177.07
244	C6H7N	3-PICOLINE	103.829	2.6047E-01	2.7853E-05	184.26
245	C6H7N	ANILINE	84.822	2.6707E-01	2.2598E-05	166.69
246	C6H10	1-HEXYNE	121.936	3.1308E-01	3.3426E-05	218.57
247	C6H10	CYCLOHEXENE	-8.701	3.7574E-01	3.5208E-05	106.86
248	C6H10	1-METHYLCYCLOPENTENE	-8.313	3.5608E-01	4.3221E-05	102.13
249	C6H10	3-METHYLCYCLOPENTENE	5.787	3.5193E-01	4.3095E-05	114.98
250	C6H10	4-METHYLCYCLOPENTENE	11.922	3.5346E-01	4.3307E-05	121.59
251	C6H10O	CYCLOHEXANONE	-234.483	4.6963E-01	3.6411E-05	-90.75
252	C6H12	1-HEXENE	-44.217	4.2734E-01	4.3352E-05	87.45
253	C6H12	2-HEXENE,CIS	-55.001	4.2475E-01	4.6828E-05	76.23
254	C6H12	2-HEXENE,TRANS	-56.244	4.3026E-01	4.4958E-05	76.44
255	C6H12	3-HEXENE,CIS	-50.434	4.3223E-01	4.6533E-05	83.01
256	C6H12	3-HEXENE,TRANS	-56.854	4.3669E-01	4.3504E-05	77.61
257	C6H12	2-METHYL-1-PENTENE	-54.752	4.3022E-01	4.1468E-05	77.61
258	C6H12	3-METHYL-1-PENTENE	-47.336	4.3630E-01	3.7470E-05	86.44
259	C6H12	4-METHYL-1-PENTENE	-46.656	4.4313E-01	4.6863E-05	90.04
260	C6H12	2-METHYL-2-PENTENE	-62.375	4.3289E-01	4.6135E-05	71.21
261	C6H12	3-METHYL-2-PENTENE,CIS	-60.369	4.3290E-01	4.6127E-05	73.22
262	C6H12	3-METHYL-2-PENTENE,TRANS	-61.309	4.2960E-01	4.6053E-05	71.30
263	C6H12	4-METHYL-2-PENTENE,CIS	-52.910	4.3887E-01	4.2824E-05	82.13
264	C6H12	4-METHYL-2-PENTENE,TRANS	-56.547	4.4368E-01	3.9806E-05	79.62
265	C6H12	2-ETHYL-1-BUTENE	-54.167	4.3620E-01	4.1384E-05	79.96
266	C6H12	2,3-DIMETHYL-1-BUTENE	-57.956	4.4708E-01	3.7750E-05	79.04
267	C6H12	3,3-DIMETHYL-1-BUTENE	-45.896	4.6814E-01	4.5620E-05	98.16
268	C6H12	2,3-DIMETHYL-2-BUTENE	-61.872	4.4549E-01	5.0110E-05	75.86
269	C6H12	CYCLOHEXANE	-127.917	5.2032E-01	4.4706E-05	31.76
270	C6H12	METHYLCYCLOPENTANE	-110.437	4.7401E-01	4.9123E-05	35.77
271	C6H12O	CYCLOHEXANOL	-299.464	5.9552E-01	3.9211E-05	-117.91
272	C6H12O	HEXANAL	-251.064	4.9255E-01	4.1576E-05	-100.12
273	C6H12S	THIACYCLOHEPTANE	-58.172	4.4956E-01	9.0710E-05	84.06
274	C6H14	HEXANE	-170.447	5.5417E-01	5.0303E-05	-0.25
275	C6H14	2-METHYLPENTANE	-177.675	5.6303E-01	4.8313E-05	-5.02
276	C6H14	3-METHYLPENTANE	-174.861	5.6271E-01	5.0351E-05	-2.13
277	C6H14	2,2-DIMETHYLBUTANE	-189.225	5.8649E-01	4.7623E-05	-9.62
278	C6H14	2,3-DIMETHYLBUTANE	-181.310	5.7783E-01	4.9722E-05	-4.10
279	C6H14O	PROPYL-ETHER	-296.085	6.2222E-01	5.0914E-05	-105.56
280	C6H14O	ISOPROPYL-ETHER	-322.050	6.5458E-01	5.0837E-05	-121.88
281	C6H14O	HEXYL-ALCOHOL	-322.918	6.0346E-01	5.1175E-05	-137.95
282	C6H14S	BUTYL-ETHYL-SULFIDE	-119.839	4.7788E-01	1.0404E-04	32.01
283	C6H14S	ISOPROPYL-SULFIDE	-136.423	5.1958E-01	9.5795E-05	27.11
284	C6H14S	METHYL-PENTYL-SULFIDE	-117.395	4.8025E-01	1.0343E-04	35.10
285	C6H14S	PROPYL-SULFIDE	-119.954	4.8210E-01	1.0475E-04	33.22
286	C6H14S	1-HEXANETHIOL	-123.627	4.7685E-01	1.0281E-04	27.82
287	C6H14S2	PROPYL-DISULFIDE	-110.285	4.5705E-01	1.2224E-04	36.99
288	C6H15N	TRIETHYLAMINE	-103.700	7.0072E-01	5.1024E-05	110.29
289	C7H5F3	A,A,A-TRIFLUOROTOLUENE	-602.334	3.0018E-01	1.5014E-05	-511.28
290	C7H5N	BENZONITRILE	217.638	1.3974E-01	1.5912E-05	260.87
291	C7H6O2	BENZOIC-ACID	-292.081	2.6249E-01	3.5028E-05	-210.41
292	C7H7F	P-FLUOROTOLUENE	-150.014	2.5689E-01	2.5593E-05	-70.88
293	C7H8	TOLUENE	47.813	2.3831E-01	3.1916E-05	122.01
294	C7H8	1,3,5-CYCLOHEPTATRIENE	179.884	2.4584E-01	2.2285E-05	255.39
295	C7H8O	M-CRESOL	-134.426	3.0573E-01	2.7772E-05	-40.54
296	C7H8O	O-CRESOL	-130.472	3.0478E-01	2.5844E-05	-37.07
297	C7H8O	P-CRESOL	-127.446	3.1458E-01	2.8223E-05	-30.88
298	C7H12	1-HEPTYNE	100.830	4.0998E-01	3.9550E-05	226.94
299	C7H14	1-HEPTENE	-65.354	5.2430E-01	4.9439E-05	95.81
300	C7H14	CYCLOHEPTANE	-124.727	6.1171E-01	5.3325E-05	63.01
301	C7H14	ETHYLCYCLOPENTANE	-131.223	5.7136E-01	5.4772E-05	44.56
302	C7H14	1,1-DIMETHYLCYCLOPENTANE	-142.804	5.9241E-01	5.2208E-05	39.04
303	C7H14	C-1,2-DIMETHYLCYCLOPENTANE	-133.964	5.8514E-01	5.2430E-05	45.73
304	C7H14	T-1,2-DIMETHYLCYCLOPENTANE	-141.075	5.8436E-01	5.2455E-05	38.37
305	C7H14	C-1,3-DIMETHYLCYCLOPENTANE	-140.261	5.8437E-01	5.2448E-05	39.20
306	C7H14	T-1,3-DIMETHYLCYCLOPENTANE	-137.981	5.8437E-01	5.2451E-05	41.46
307	C7H14	METHYLCYCLOHEXANE	-160.038	6.1255E-01	4.6303E-05	27.28
308	C7H14O	HEPTANAL	-267.231	5.8999E-01	4.7332E-05	-86.65
309	C7H16	HEPTANE	-191.520	6.5052E-01	5.6444E-05	7.99
310	C7H16	2-METHYLHEXANE	-198.645	6.5837E-01	5.6475E-05	3.22
311	C7H16	3-METHYLHEXANE	-196.032	6.5427E-01	5.6454E-05	4.60
312	C7H16	3-ETHYLPENTANE	-193.374	6.6687E-01	5.6450E-05	11.00
313	C7H16	2,2-DIMETHYLPENTANE	-209.894	6.8563E-01	5.6352E-05	0.08
314	C7H16	2,3-DIMETHYLPENTANE	-203.028	6.6456E-01	5.6286E-05	0.67
315	C7H16	2,4-DIMETHYLPENTANE	-205.762	6.8189E-01	5.6332E-05	3.10
316	C7H16	3,3-DIMETHYLPENTANE	-205.327	6.7887E-01	5.6327E-05	2.64
317	C7H16	2,2,3-TRIMETHYLBUTANE	-209.101	6.9811E-01	5.2621E-05	4.27
318	C7H16O	ISOPROPYL-TERT-BUTYL-ETHER	-361.844	7.6268E-01	5.6918E-05	-128.83
319	C7H16O	HEPTYL-ALCOHOL	-338.701	7.0060E-01	5.7147E-05	-124.18
320	C7H16S	BUTYL-PROPYL-SULFIDE	-140.231	5.6947E-01	1.1450E-04	39.87
321	C7H16S	ETHYL-PENTYL-SULFIDE	-140.038	5.7058E-01	1.1447E-04	40.38
322	C7H16S	HEXYL-METHYL-SULFIDE	-137.588	5.7293E-01	1.1389E-04	43.47
323	C7H16S	1-HEPTANETHIOL	-143.858	5.6969E-01	1.1320E-04	36.19
324	C8H6	ETHYNYLBENZENE	326.263	1.1297E-01	1.8500E-05	361.75
325	C8H8	STYRENE	145.657	2.1917E-01	2.8490E-05	213.80
326	C8H8	1,3,5,7-CYCLOOCTATETRAENE	296.084	2.3877E-01	2.6787E-05	369.91
327	C8H10	ETHYLBENZENE	27.421	3.3327E-01	3.8542E-05	130.58
328	C8H10	M-XYLENE	15.063	3.3452E-01	4.1387E-05	118.87
329	C8H10	O-XYLENE	17.048	3.3940E-01	3.9428E-05	122.09
330	C8H10	P-XYLENE	15.763	3.3952E-01	4.2301E-05	121.13
331	C8H14	1-OCTYNE	79.739	5.0705E-01	4.5503E-05	235.39
332	C8H16	1-OCTENE	-86.500	6.2135E-01	5.5457E-05	104.22
333	C8H16	CYCLOOCTANE	-131.710	7.2244E-01	6.2236E-05	89.91
334	C8H16	PROPYLCYCLOPENTANE	-152.696	6.6824E-01	6.0934E-05	52.59
335	C8H16	ETHYLCYCLOHEXANE	-177.580	7.0980E-01	5.1198E-05	39.25
336	C8H16	1,1-DIMETHYLCYCLOHEXANE	-187.269	7.2867E-01	5.1482E-05	35.23
337	C8H16	C-1,2-DIMETHYLCYCLOHEXANE	-178.140	7.1809E-01	5.1867E-05	41.21
338	C8H16	T-1,2-DIMETHYLCYCLOHEXANE	-185.997	7.2249E-01	4.9658E-05	34.48
339	C8H16	C-1,3-DIMETHYLCYCLOHEXANE	-190.817	7.2267E-01	5.1077E-05	29.83
340	C8H16	T-1,3-DIMETHYLCYCLOHEXANE	-182.416	7.1581E-01	5.2435E-05	36.32
341	C8H16	C-1,4-DIMETHYLCYCLOHEXANE	-182.489	7.2157E-01	5.2435E-05	37.95
342	C8H16	T-1,4-DIMETHYLCYCLOHEXANE	-190.646	7.2867E-01	5.0049E-05	31.71
343	C8H16O	OCTANAL	-293.423	6.8704E-01	5.3338E-05	-83.30
344	C8H18	OCTANE	-212.692	7.4774E-01	6.2361E-05	16.40
345	C8H18	2-METHYLHEPTANE	-219.792	7.5940E-01	6.2231E-05	12.76
346	C8H18	3-METHYLHEPTANE	-216.883	7.5284E-01	6.2428E-05	13.72
347	C8H18	4-METHYLHEPTANE	-216.353	7.6119E-01	6.2325E-05	16.74
348	C8H18	3-ETHYLHEXANE	-215.139	7.5633E-01	6.2330E-05	16.53
349	C8H18	2,2-DIMETHYLHEXANE	-220.039	7.8345E-01	6.2253E-05	10.71
350	C8H18	2,3-DIMETHYLHEXANE	-218.217	7.7062E-01	6.2282E-05	17.70
351	C8H18	2,4-DIMETHYLHEXANE	-223.697	7.6894E-01	6.2289E-05	11.72
352	C8H18	2,5-DIMETHYLHEXANE	-226.952	7.7568E-01	6.2197E-05	10.46
353	C8H18	3,3-DIMETHYLHEXANE	-224.411	7.7653E-01	6.2269E-05	13.26
354	C8H18	3,4-DIMETHYLHEXANE	-217.260	7.6617E-01	6.2351E-05	17.32
355	C8H18	3-ETHYL-2-METHYLPENTANE	-215.532	7.7359E-01	6.2197E-05	21.25
356	C8H18	3-ETHYL-3-METHYLPENTANE	-219.251	7.8158E-01	6.2315E-05	19.92
357	C8H18	2,2,3-TRIMETHYLPENTANE	-224.335	7.8913E-01	6.2502E-05	17.11
358	C8H18	2,2,4-TRIMETHYLPENTANE	-228.383	7.9125E-01	6.2364E-05	13.68
359	C8H18	2,3,3-TRIMETHYLPENTANE	-220.671	7.8284E-01	6.2446E-05	18.91
360	C8H18	2,3,4-TRIMETHYLPENTANE	-221.742	7.8655E-01	6.2266E-05	18.91
361	C8H18	2,2,3,3-TETRAMETHYLBUTANE	-231.148	8.3203E-01	5.0497E-05	22.01
362	C8H18O	BUTYL-ETHER	-337.796	8.1490E-01	6.4263E-05	-88.53
363	C8H18O	SEC-BUTYL-ETHER	-364.965	8.5433E-01	6.2752E-05	-104.06
364	C8H18O	TERT-BUTYL-ETHER	-369.106	8.8957E-01	6.2818E-05	-97.70
365	C8H18O	OCTYL-ALCOHOL	-361.386	7.9753E-01	6.3199E-05	-117.36
366	C8H18S	BUTYL-SULFIDE	-161.106	6.6757E-01	1.2527E-04	49.20
367	C8H18S	ETHYL-HEXYL-SULFIDE	-160.100	6.6283E-01	1.2547E-04	48.83
368	C8H18S	HEPTYL-METHYL-SULFIDE	-157.568	6.6496E-01	1.2493E-04	51.92
369	C8H18S	PENTYL-PROPYL-SULFIDE	-160.310	6.6161E-01	1.2550E-04	48.24
370	C8H18S	1-OCTANETHIOL	-163.961	6.6230E-01	1.2366E-04	44.64
371	C8H18S2	BUTY-DISULFIDE	-150.651	6.4275E-01	1.4278E-04	53.85
372	C9H10	ALPHA-METHYLSTYRENE	111.072	3.1472E-01	3.7121E-05	208.53
373	C9H10	PROPENYLBENZENE,CIS	119.443	3.1471E-01	3.7129E-05	216.90
374	C9H10	PROPENYLBENZENE,TRANS	115.154	3.1893E-01	3.5506E-05	213.72
375	C9H10	M-METHYLSTYRENE	113.573	3.0888E-01	3.7107E-05	209.28
376	C9H10	O-METHYLSTYRENE	116.520	3.1469E-01	3.7144E-05	213.97
377	C9H10	P-METHYLSTYRENE	112.745	3.1472E-01	3.7119E-05	210.20
378	C9H12	PROPYLBENZENE	4.889	4.2937E-01	4.4012E-05	137.24
379	C9H12	CUMENE	0.983	4.4175E-01	4.3406E-05	136.98
380	C9H12	M-ETHYLTOLUENE	-4.705	4.2485E-01	4.5613E-05	126.44
381	C9H12	O-ETHYLTOLUENE	-1.301	4.2958E-01	4.3769E-05	131.08
382	C9H12	P-ETHYLTOLUENE	-5.947	4.2950E-01	4.6751E-05	126.69
383	C9H12	1,2,3-TRIMETHYLBENZENE	-11.858	4.4140E-01	4.9389E-05	124.56
384	C9H12	1,2,4-TRIMETHYLBENZENE	-16.358	4.3119E-01	4.8564E-05	116.94
385	C9H12	MESITYLENE	-18.595	4.4166E-01	4.9679E-05	117.95
386	C9H16	1-NONYNE	58.588	6.0406E-01	5.1578E-05	243.76
387	C9H18	1-NONENE	-107.582	7.1838E-01	6.1441E-05	112.68
388	C9H18	BUTYLCYCLOPENTANE	-173.390	7.6514E-01	6.7065E-05	61.38
389	C9H18	PROPYLCYCLOHEXANE	-199.501	8.0874E-01	5.6176E-05	47.32
390	C9H18	C-C-135TRIMETHYLCYCLOHEXANE	-222.259	8.4009E-01	5.5762E-05	33.89
391	C9H18	C-T-135TRIMETHYLCYCLOHEXANE	-212.955	8.2810E-01	5.8630E-05	39.87
392	C9H18O	NONANAL	-314.560	7.8403E-01	5.9438E-05	-74.94
393	C9H20	NONANE	-233.826	8.4477E-01	6.8451E-05	24.81
394	C9H20	2-METHYLOCTANE	-240.805	8.5474E-01	6.6289E-05	20.59
395	C9H20	3-METHYLOCTANE	-238.219	8.4955E-01	6.6996E-05	21.71
396	C9H20	4-METHYLOCTANE	-238.219	8.4955E-01	6.6996E-05	21.71
397	C9H20	3-ETHYLHEPTANE	-235.493	8.5556E-01	6.7981E-05	26.32
398	C9H20	4-ETHYLHEPTANE	-235.493	8.5556E-01	6.7981E-05	26.32
399	C9H20	2,2-DIMETHYLHEPTANE	-251.912	8.8046E-01	6.1573E-05	16.74
400	C9H20	2,3-DIMETHYLHEPTANE	-240.580	8.6274E-01	6.7176E-05	23.30
401	C9H20	2,4-DIMETHYLHEPTANE	-245.667	8.6328E-01	6.7859E-05	18.45
402	C9H20	2,5-DIMETHYLHEPTANE	-245.667	8.6328E-01	6.7859E-05	18.45
403	C9H20	2,6-DIMETHYLHEPTANE	-248.402	8.7460E-01	6.6904E-05	19.00
404	C9H20	3,3-DIMETHYLHEPTANE	-246.821	8.7164E-01	6.2519E-05	19.29
405	C9H20	3,4-DIMETHYLHEPTANE	-237.951	8.6040E-01	6.7955E-05	25.31
406	C9H20	3,5-DIMETHYLHEPTANE	-243.061	8.6678E-01	6.8579E-05	22.18
407	C9H20	4,4-DIMETHYLHEPTANE	-246.853	8.7750E-01	6.2463E-05	21.00
408	C9H20	3-ETHYL-2-METHYLHEXANE	-237.903	8.6316E-01	6.8037E-05	26.19
409	C9H20	4-ETHYL-2-METHYLHEXANE	-243.011	8.6950E-01	6.8697E-05	23.05
410	C9H20	3-ETHYL-3-METHYLHEXANE	-241.791	8.7215E-01	6.3284E-05	24.56
411	C9H20	3-ETHYL-4-METHYLHEXANE	-235.257	8.6369E-01	6.8766E-05	29.08
412	C9H20	2,2,3-TRIMETHYLHEXANE	-246.598	8.8845E-01	6.2515E-05	24.52
413	C9H20	2,2,4-TRIMETHYLHEXANE	-248.840	8.8895E-01	6.3241E-05	22.51
414	C9H20	2,2,5-TRIMETHYLHEXANE	-259.495	8.9459E-01	6.2167E-05	13.43
415	C9H20	2,3,3-TRIMETHYLHEXANE	-244.225	8.8514E-01	6.2489E-05	25.90
416	C9H20	2,3,4-TRIMETHYLHEXANE	-240.368	8.7376E-01	6.8017E-05	26.90
417	C9H20	2,3,5-TRIMETHYLHEXANE	-248.145	8.8262E-01	6.7777E-05	21.76
418	C9H20	2,4,4-TRIMETHYLHEXANE	-246.460	8.8561E-01	6.3235E-05	23.89
419	C9H20	3,3,4-TRIMETHYLHEXANE	-241.552	8.7981E-01	6.3300E-05	27.07
420	C9H20	3,3-DIETHYLPENTANE	-237.693	8.9338E-01	6.4026E-05	35.06
421	C9H20	3-ETHYL-2,2-DIMETHYLPENTANE	-243.872	8.9430E-01	6.3760E-05	29.12
422	C9H20	3-ETHYL-2,3-DIMETHYLPENTANE	-239.241	8.8583E-01	6.3120E-05	31.17
423	C9H20	3-ETHYL-2,4-DIMETHYLPENTANE	-240.323	8.8226E-01	6.8132E-05	29.50
424	C9H20	2,2,3,3-TRIMETHYLPENTANE	-242.926	9.1022E-01	5.8406E-05	34.31
425	C9H20	2,2,3,4-TETRAMETHYLPENTANE	-242.527	9.0198E-01	6.2433E-05	32.64
426	C9H20	2,2,4,4-TETRAMETHYLPENTANE	-247.825	9.2587E-01	5.7635E-05	34.02
427	C9H20	2,3,3,4-TETRAMETHYLPENTANE	-241.799	9.0451E-01	6.2351E-05	34.10
428	C9H20O	NONYL-ALCOHOL	-391.755	8.9463E-01	6.9190E-05	-118.20
429	C9H20S	BUTYL-PENTYL-SULFIDE	-181.275	7.5451E-01	1.3571E-04	55.90
430	C9H20S	ETHYL-HEPTYL-SULFIDE	-180.361	7.5587E-01	1.3553E-04	57.20
431	C9H20S	HEXYL-PROPYL-SULFIDE	-180.488	7.5455E-01	1.3567E-04	56.69
432	C9H20S	METHYL-OCTYL-SULFIDE	-177.894	7.5828E-01	1.3475E-04	60.33
433	C9H20S	1-NONANETHIOL	-184.234	7.5533E-01	1.3380E-04	53.01
434	C10H8	NAPHTHALENE	148.988	2.4014E-01	3.0705E-05	223.59
435	C10H8	AZULENE	277.714	2.3826E-01	3.1796E-05	351.87
436	C10H14	BUTYLBENZENE	-17.190	5.2633E-01	5.0190E-05	144.68
437	C10H14	M-DIETHYLBENZENE	-25.143	5.2637E-01	4.9852E-05	136.69
438	C10H14	O-DIETHYLBENZENE	-21.957	5.3091E-01	4.8193E-05	141.08
439	C10H14	P-DIETHYLBENZENE	-25.535	5.3121E-01	5.0922E-05	137.86
440	C10H14	1,2,3,4-TETRAMETHYLBENZENE	-44.515	5.4762E-01	4.7618E-05	123.43
441	C10H14	1,2,3,5-TETRAMETHYLBENZENE	-47.443	5.4079E-01	5.0474E-05	118.74
442	C10H14	1,2,4,5-TETRAMETHYLBENZENE	-47.801	5.4403E-01	5.1676E-05	119.45
443	C10H18	1-DECYNE	37.488	7.0119E-01	5.7516E-05	252.21
444	C10H18	DECAHYDRONAPHTHALENE,CIS	-175.788	8.5412E-01	6.9065E-05	85.81
445	C10H18	DECAHYDRONAPHTHALENE,TRANS	-189.001	8.5677E-01	6.9466E-05	73.43
446	C10H20	1-DECENE	-128.709	8.1530E-01	6.7574E-05	121.04
447	C10H20	1-CYCLOPENTYLPENTANE	-194.532	8.6222E-01	7.3010E-05	69.79
448	C10H20	BUTYLCYCLOHEXANE	-219.884	9.0572E-01	6.2305E-05	56.44
449	C10H20O	DECANAL	-335.674	8.8103E-01	6.5416E-05	-66.53
450	C10H22	DECANE	-255.000	9.4201E-01	7.4254E-05	33.22
451	C10H22	2-METHYLNONANE	-261.869	9.5206E-01	7.1758E-05	29.08
452	C10H22	3-METHYLNONANE	-259.232	9.4674E-01	7.2527E-05	30.21
453	C10H22	4-METHYLNONANE	-259.232	9.4674E-01	7.2527E-05	30.21
454	C10H22	5-METHYLNONANE	-259.270	9.5261E-01	7.2471E-05	31.92
455	C10H22	3-ETHYLOCTANE	-256.591	9.5302E-01	7.3335E-05	34.81
456	C10H22	4-ETHYLOCTANE	-256.563	9.4713E-01	7.3410E-05	33.10
457	C10H22	2,2-DIMETHYLOCTANE	-272.907	9.7753E-01	6.7222E-05	25.23
458	C10H22	2,3-DIMETHYLOCTANE	-266.771	9.6074E-01	7.3210E-05	26.94
459	C10H22	2,4-DIMETHYLOCTANE	-261.653	9.6011E-01	7.2592E-05	31.80
460	C10H22	2,5-DIMETHYLOCTANE	-266.771	9.6074E-01	7.3210E-05	26.94
461	C10H22	2,6-DIMETHYLOCTANE	-266.771	9.6074E-01	7.3210E-05	26.94
462	C10H22	2,7-DIMETHYLOCTANE	-269.396	9.7167E-01	7.2527E-05	27.49
463	C10H22	3,3-DIMETHYLOCTANE	-267.928	9.6911E-01	6.7859E-05	27.78
464	C10H22	3,4-DIMETHYLOCTANE	-259.027	9.5779E-01	7.3332E-05	33.81
465	C10H22	3,5-DIMETHYLOCTANE	-264.140	9.5839E-01	7.3992E-05	28.95
466	C10H22	3,6-DIMETHYLOCTANE	-264.093	9.6400E-01	7.4100E-05	30.67
467	C10H22	4,4-DIMETHYLOCTANE	-267.928	9.6911E-01	6.7859E-05	27.78
468	C10H22	4,5-DIMETHYLOCTANE	-258.993	9.6344E-01	7.3443E-05	35.52
469	C10H22	4-PROPYLHEPTANE	-256.533	9.6193E-01	7.3483E-05	37.53
470	C10H22	4-ISOPROPYLHEPTANE	-256.743	9.6635E-01	7.3427E-05	38.66

Continued

NO.	FORMULA	NAME	A	B	C	DEL GF @298K
471	C10H22	3-ETHYL-2-METHYLHEPTANE	-258.970	9.6045E-01	7.3515E-05	34.69
472	C10H22	4-ETHYL-2-METHYLHEPTANE	-264.077	9.6109E-01	7.4107E-05	29.83
473	C10H22	5-ETHYL-2-METHYLHEPTANE	-264.106	9.6694E-01	7.4061E-05	31.55
474	C10H22	3-ETHYL-3-METHYLHEPTANE	-262.888	9.6960E-01	6.8641E-05	33.05
475	C10H22	4-ETHYL-3-METHYLHEPTANE	-256.382	9.5829E-01	7.4126E-05	36.69
476	C10H22	3-ETHYL-5-METHYLHEPTANE	-261.414	9.6136E-01	7.5079E-05	32.68
477	C10H22	3-ETHYL-4-METHYLHEPTANE	-256.320	9.6100E-01	7.4238E-05	37.57
478	C10H22	4-ETHYL-4-METHYLHEPTANE	-262.888	9.6960E-01	6.8641E-05	33.05
479	C10H22	2,2,3-TRIMETHYLHEPTANE	-267.615	9.8561E-01	6.8083E-05	33.01
480	C10H22	2,2,4-TRIMETHYLHEPTANE	-269.875	9.8622E-01	6.8723E-05	31.00
481	C10H22	2,2,5-TRIMETHYLHEPTANE	-277.782	9.8622E-01	6.8723E-05	23.10
482	C10H22	2,2,6-TRIMETHYLHEPTANE	-280.476	9.9171E-01	6.7751E-05	21.97
483	C10H22	2,3,3-TRIMETHYLHEPTANE	-265.181	9.8212E-01	6.8178E-05	34.43
484	C10H22	2,3,4-TRIMETHYLHEPTANE	-261.391	9.7099E-01	7.3509E-05	35.40
485	C10H22	2,3,5-TRIMETHYLHEPTANE	-266.466	9.7144E-01	7.4281E-05	30.54
486	C10H22	2,3,6-TRIMETHYLHEPTANE	-269.149	9.7393E-01	7.3404E-05	28.53
487	C10H22	2,4,4-TRIMETHYLHEPTANE	-267.448	9.8275E-01	6.8799E-05	32.43
488	C10H22	2,4,5-TRIMETHYLHEPTANE	-266.466	9.7144E-01	7.4281E-05	30.54
489	C10H22	2,4,6-TRIMETHYLHEPTANE	-259.166	9.8025E-01	7.4100E-05	40.46
490	C10H22	2,5,5-TRIMETHYLHEPTANE	-275.356	9.8275E-01	6.8799E-05	24.52
491	C10H22	3,3,4-TRIMETHYLHEPTANE	-262.647	9.7725E-01	6.8661E-05	35.56
492	C10H22	3,3,5-TRIMETHYLHEPTANE	-264.902	9.7782E-01	6.9318E-05	33.56
493	C10H22	3,4,4-TRIMETHYLHEPTANE	-262.647	9.7725E-01	6.8661E-05	35.56
494	C10H22	2,3,5-TRIMETHYLHEPTANE	-259.802	9.7161E-01	7.5693E-05	38.24
495	C10H22	3-ISOPROPYL-2-METHYLHEXANE	-261.387	9.7967E-01	7.3499E-05	37.99
496	C10H22	3,3-DIETHYLHEXANE	-257.797	9.7908E-01	6.9505E-05	41.05
497	C10H22	3,4-DIETHYLHEXANE	-253.621	9.7301E-01	7.5062E-05	43.93
498	C10H22	3-ETHYL-2,2-DIMETHYLHEXANE	-264.982	9.8620E-01	6.8786E-05	35.90
499	C10H22	4-ETHYL-2,2-DIMETHYLHEXANE	-267.225	9.9254E-01	6.9429E-05	35.65
500	C10H22	3-ETHYL-2,3-DIMETHYLHEXANE	-260.267	9.7727E-01	6.8648E-05	37.95
551	C12H12	1,2-DIMETHYLNAPHTHALENE	80.611	4.4220E-01	3.8339E-05	216.23
552	C12H12	1,3-DIMETHYLNAPHTHALENE	78.976	4.3881E-01	3.9571E-05	213.72
553	C12H12	1,4-DIMETHYLNAPHTHALENE	79.522	4.4807E-01	3.8242E-05	216.90
554	C12H12	1,5-DIMETHYLNAPHTHALENE	78.821	4.4803E-01	3.8272E-05	216.19
555	C12H12	1,6-DIMETHYLNAPHTHALENE	79.690	4.3879E-01	3.9579E-05	214.63
556	C12H12	1,7-DIMETHYLNAPHTHALENE	78.976	4.3881E-01	3.9571E-05	213.72
557	C12H12	2,3-DIMETHYLNAPHTHALENE	81.060	4.3524E-01	4.2654E-05	215.02
558	C12H12	2,6-DIMETHYLNAPHTHALENE	79.922	4.3839E-01	4.0694E-05	214.64
559	C12H12	2,7-DIMETHYLNAPHTHALENE	79.918	4.3842E-01	4.0642E-05	214.64
560	C12H18	HEXYLBENZENE	-59.463	7.1997E-01	6.2172E-05	161.34
561	C12H18	1,2,3-TRIETHYLBENZENE	-71.837	7.2867E-01	6.2504E-05	151.54
562	C12H18	1,2,4-TRIETHYLBENZENE	-72.938	7.1000E-01	6.8084E-05	145.23
563	C12H18	1,3,5-TRIETHYLBENZENE	-78.848	7.2900E-01	6.2716E-05	144.68
564	C12H18	HEXAMETHYLBENZENE	-109.218	7.8642E-01	5.0247E-05	130.21
565	C12H22	1-DODECYNE	-4.724	8.9500E-01	6.9758E-05	268.99
566	C12H24	1-DODECENE	-178.907	1.0093E+00	7.9654E-05	137.90
567	C12H24	1-CYCLOPENTYLHEPTANE	-236.801	1.0564E+00	8.5011E-05	86.61
568	C12H24	1-CYCLOHEXYLHEXANE	-262.182	1.1000E+00	7.4071E-05	73.26
569	C12H26	DODECANE	-297.182	1.1359E+00	8.6457E-05	50.04
570	C12H26O	DODECYL-ALCOHOL	-449.239	1.1858E+00	8.7192E-05	-87.07
571	C12H26S	BUTYL-OCTYL-SULFIDE	-241.769	1.0327E+00	1.6697E-04	81.17
572	C12H26S	DECYL-ETHYL-SULFIDE	-242.383	1.0341E+00	1.6662E-04	80.92
573	C12H26S	HEXYL-SULFIDE	-241.877	1.0389E+00	1.6649E-04	82.89
574	C12H26S	METHYL-UNDECYL-SULFIDE	-238.536	1.0370E+00	1.6539E-04	85.52
575	C12H26S	NONYL-PROPYL-SULFIDE	-241.027	1.0327E+00	1.6692E-04	81.92
576	C12H26S	1-DODECANETHIOL	-244.797	1.0337E+00	1.6475E-04	78.26
577	C12H26S2	HEXYL-DISULFIDE	-231.339	1.0136E+00	1.8450E-04	87.49
578	C13H14	1-PROPYLNAPHTHALENE	71.181	5.2690E-01	4.3941E-05	232.63
579	C13H14	2-PROPYLNAPHTHALENE	70.476	5.2339E-01	4.5280E-05	231.00
580	C13H14	2ETHYL-3-METHYLNAPHTHALENE	62.759	5.2530E-01	4.7025E-05	224.01
581	C13H14	2ETHYL-6-METHYLNAPHTHALENE	58.499	5.2712E-01	4.6332E-05	220.20
582	C13H14	2ETHYL-7-METHYLNAPHTHALENE	58.499	5.2712E-01	4.6332E-05	220.20
583	C13H20	1-PHENYLHEPTANE	-80.556	8.1688E-01	6.8286E-05	169.74
584	C13H24	1-TRIDECYNE	-25.829	9.9206E-01	7.5746E-05	277.44
501	C10H22	4-ETHYL-2,3-DIMETHYLHEXANE	-258.811	9.7449E-01	7.4202E-05	39.12
502	C10H22	3-ETHYL-2,4-DIMETHYLHEXANE	-258.787	9.7149E-01	7.4304E-05	38.24
503	C10H22	4-ETHYL-2,4-DIMETHYLHEXANE	-262.418	9.8330E-01	6.9521E-05	37.70
504	C10H22	3-ETHYL-2,5-DIMETHYLHEXANE	-266.527	9.7459E-01	7.4067E-05	31.42
505	C10H22	4-ETHYL-3,3-DIMETHYLHEXANE	-259.929	9.8334E-01	6.9567E-05	40.21
506	C10H22	3-ETHYL-3,4-DIMETHYLHEXANE	-257.579	9.7763E-01	6.9541E-05	40.84
507	C10H22	2,2,3,3-TETRAMETHYLHEXANE	-264.021	1.0077E+00	6.3741E-05	42.80
508	C10H22	2,2,3,4-TETRAMETHYLHEXANE	-259.481	9.9664E-01	6.8878E-05	44.56
509	C10H22	2,2,3,5-TETRAMETHYLHEXANE	-275.197	9.9984E-01	6.8575E-05	29.75
510	C10H22	2,2,4,4-TETRAMETHYLHEXANE	-263.859	1.0089E+00	6.3813E-05	43.35
511	C10H22	2,2,4,5-TETRAMETHYLHEXANE	-272.355	9.9985E-01	6.8569E-05	32.59
512	C10H22	2,2,5,5-TETRAMETHYLHEXANE	-291.593	1.0233E+00	6.2952E-05	19.83
513	C10H22	2,3,3,4-TETRAMETHYLHEXANE	-260.022	9.9071E-01	6.8648E-05	42.22
514	C10H22	2,3,3,5-TETRAMETHYLHEXANE	-264.912	9.9652E-01	6.8562E-05	39.04
515	C10H22	2,3,4,4-TETRAMETHYLHEXANE	-257.185	9.9074E-01	6.8625E-05	45.06
516	C10H22	2,3,4,5-TETRAMETHYLHEXANE	-263.908	9.9031E-01	7.3463E-05	38.66
517	C10H22	3,3,4,4-TETRAMETHYLHEXANE	-258.982	1.0048E+00	6.4558E-05	47.07
518	C10H22	24DIMETHYL3ISOPROPYLPENTANE	-264.215	1.0048E+00	6.8707E-05	42.26
519	C10H22	33-DIETHYL-2-METHYLPENTANE	-255.118	9.9226E-01	6.9725E-05	47.70
520	C10H22	3ETHYL-223TRIMETHYLPENTANE	-258.971	1.0024E+00	6.4555E-05	46.36
521	C10H22	3ETHYL-224TRIMETHYLPENTANE	-259.533	1.0062E+00	6.8727E-05	47.32
522	C10H22	3ETHYL-234TRIMETHYLPENTANE	-257.589	9.9632E-01	6.8759E-05	46.32
523	C10H22	22334-PENTAMETHYLPENTANE	-253.281	1.0201E+00	6.4778E-05	57.36
524	C10H22	22344-PENTAMETHYLPENTANE	-253.379	1.0306E+00	6.3360E-05	60.25
525	C10H22O	DECYL-ALCOHOL	-408.594	9.9155E-01	7.5283E-05	-105.52
526	C10H22S	BUTYL-HEXYL-SULFIDE	-201.497	8.4742E-01	1.4603E-04	64.31
527	C10H22S	ETHYL-OCTYL-SULFIDE	-200.446	8.4814E-01	1.4635E-04	65.61
528	C10H22S	HEPTYL-PROPYL-SULFIDE	-200.752	8.4746E-01	1.4599E-04	65.06
529	C10H22S	METHYL-NONYL-SULFIDE	-198.094	8.5098E-01	1.4518E-04	68.70
530	C10H22S	PENTYL-SULFIDE	-201.402	8.5291E-01	1.4621E-04	66.07
531	C10H22S	1-DECANETHIOL	-204.389	8.4798E-01	1.4421E-04	61.42
532	C10H22S2	PENTYL-DISULFIDE	-190.970	8.2801E-01	1.6386E-04	70.67
533	C11H10	1-METHYLNAPHTHALENE	114.458	3.3490E-01	3.4180E-05	217.69
534	C11H10	2-METHYLNAPHTHALENE	113.834	3.3151E-01	3.5442E-05	216.15
535	C11H16	PENTYLBENZENE	-38.343	6.2290E-01	5.6186E-05	152.93
536	C11H16	PENTAMETHYLBENZENE	-77.647	6.5761E-01	4.9942E-05	123.34
537	C11H20	1-UNDECYNE	16.390	7.9808E-01	6.3658E-05	260.62
538	C11H22	1-UNDECENE	-149.838	9.1236E-01	7.3538E-05	129.45
539	C11H22	1-CYCLOPENTYLHEXANE	-215.718	9.5953E-01	7.8827E-05	78.20
540	C11H22	PENTYLCYCLOHEXANE	-241.092	1.0031E+00	6.7958E-05	64.85
541	C11H24	UNDECANE	-276.105	1.0389E+00	8.0406E-05	41.59
542	C11H24O	UNDECYL-ALCOHOL	-428.070	1.0886E+00	8.1234E-05	-95.44
543	C11H24S	BUTYL-HEPTYL-SULFIDE	-221.656	9.4009E-01	1.5642E-04	72.72
544	C11H24S	DECYL-METHYL-SULFIDE	-218.271	9.4391E-01	1.5535E-04	77.15
545	C11H24S	ETHYL-NONYL-SULFIDE	-220.622	9.4107E-01	1.5652E-04	74.06
546	C11H24S	OCTYL-PROPYL-SULFIDE	-220.786	9.4013E-01	1.5638E-04	73.60
547	C11H24S	1-UNDECANETHIOL	-224.542	9.4068E-01	1.5465E-04	69.83
548	C12H10	BIPHENYL	179.415	3.2590E-01	3.5313E-05	280.08
549	C12H12	1-ETHYLNAPHTHALENE	93.648	4.3103E-01	3.8318E-05	225.98
550	C12H12	2-ETHYLNAPHTHALENE	93.053	4.2755E-01	3.9627E-05	224.43
585	C13H26	1-TRIDECENE	-192.059	1.1064E+00	8.5626E-05	146.27
586	C13H26	1-CYCLOPENTYLOCTANE	-257.926	1.1536E+00	9.0881E-05	95.06
587	C13H26	1-CYCLOHEXYLHEPTANE	-283.301	1.1970E+00	8.0042E-05	81.67
588	C13H28	TRIDECANE	-318.273	1.2328E+00	9.2592E-05	58.45
589	C13H28O	1-TRIDECANOL	-470.339	1.2840E+00	9.3318E-05	-78.28
590	C13H28S	BUTYL-NONYL-SULFIDE	-261.912	1.1252E+00	1.7759E-04	89.54
591	C13H28S	DECYL-PROPYL-SULFIDE	-261.150	1.1251E+00	1.7763E-04	90.29
592	C13H28S	DODECYL-METHYL-SULFIDE	-258.629	1.1295E+00	1.7609E-04	93.97
593	C13H28S	ETHYL-UNDECYL-SULFIDE	-260.976	1.1265E+00	1.7738E-04	90.88
594	C13H28S	1-TRIDECANETHIOL	-264.946	1.1264E+00	1.7521E-04	86.65
595	C14H16	1-BUTYLNAPHTHALENE	49.101	6.2380E-01	5.0256E-05	240.08
596	C14H16	2-BUTYLNAPHTHALENE	48.475	6.2035E-01	5.1496E-05	238.53
597	C14H22	1-PHENYLOCTANE	-101.612	9.1381E-01	7.4333E-05	178.20
598	C14H22	1,2,3,4-TETRAETHYLBENZENE	-128.011	9.3083E-01	6.4969E-05	155.94
599	C14H22	1,2,3,5-TETRAETHYLBENZENE	-127.656	9.2614E-01	6.7695E-05	154.56
600	C14H22	1,2,4,5-TETRAETHYLBENZENE	-127.872	9.2707E-01	6.9124E-05	155.35
601	C14H26	1-TETRADECYNE	-46.990	1.0891E+00	8.1802E-05	285.81
602	C14H28	1-TETRADECENE	-213.140	1.2035E+00	9.1571E-05	154.77
603	C14H28	1-CYCLOPENTYLNONANE	-279.030	1.2505E+00	9.7036E-05	103.43
604	C14H28	1-CYCLOHEXYLOCTANE	-304.390	1.2940E+00	8.6187E-05	90.08
605	C14H30	TETRADECANE	-339.495	1.3301E+00	9.8399E-05	66.82
606	C14H30O	1-TETRADECANOL	-491.525	1.3812E+00	9.9188E-05	-69.87
607	C14H30S	BUTYL-DECYL-SULFIDE	-282.126	1.2181E+00	1.8779E-04	97.95
608	C14H30S	DODECYL-ETHYL-SULFIDE	-281.237	1.2195E+00	1.8745E-04	99.24
609	C14H30S	HEPTYL-SULFIDE	-282.102	1.2238E+00	1.8786E-04	99.70
610	C14H30S	METHYL-TRIDECYL-SULFIDE	-278.793	1.2219E+00	1.8683E-04	102.34
611	C14H30S	PROPYL-UNDECYL-SULFIDE	-281.344	1.2181E+00	1.8773E-04	98.74
612	C14H30S	1-TETRADECANETHIOL	-285.169	1.2193E+00	1.8537E-04	95.06
613	C14H30S2	HEPTYL-DISULFIDE	-271.597	1.1987E+00	2.0566E-04	104.31
614	C15H18	1-PENTYLNAPHTHALENE	27.930	7.2052E-01	5.6005E-05	248.32
615	C15H18	2-PENTYLNAPHTHALENE	27.301	7.1700E-01	5.7364E-05	246.77
616	C15H24	1-PHENYLNONANE	-122.814	1.0110E+00	8.0315E-05	186.56
617	C15H28	1-PENTADECYNE	-68.040	1.1860E+00	8.7866E-05	294.26
618	C15H30	1-PENTADECENE	-234.403	1.3006E+00	9.7536E-05	163.05
619	C15H30	1-CYCLOPENTYLDECANE	-300.184	1.3476E+00	1.0295E-04	111.84
620	C15H30	1-CYCLOHEXYLNONANE	-325.560	1.3912E+00	9.2165E-05	98.49
621	C15H32	PENTADECANE	-360.562	1.4269E+00	1.0458E-04	75.23
622	C15H32O	1-PENTADECANOL	-512.580	1.4780E+00	1.0540E-04	-61.46
623	C15H32S	BUTYL-UNDECYL-SULFIDE	-302.378	1.3111E+00	1.9792E-04	106.36
624	C15H32S	DODECYL-PROPYL-SULFIDE	-301.620	1.3111E+00	1.9794E-04	107.11
625	C15H32S	ETHYL-TRIDECYL-SULFIDE	-301.464	1.3125E+00	1.9758E-04	107.65
626	C15H32S	METHYL-TETRADECYL-SULFIDE	-298.940	1.3145E+00	1.9728E-04	110.75
627	C15H32S	1-PENTADECANETHIOL	-305.323	1.3120E+00	1.9578E-04	103.47
628	C16H26	1-PHENYLDECANE	-143.980	1.1082E+00	8.6141E-05	194.97
629	C16H26	PENTAETHYLBENZENE	-181.006	1.1365E+00	7.1696E-05	164.98
630	C16H30	1-HEXADECYNE	-89.177	1.2831E+00	9.3850E-05	302.67
631	C16H32	1-HEXADECENE	-255.460	1.3976E+00	1.0363E-04	171.50
632	C16H32	1-CYCLOPENTYLUNDECANE	-321.252	1.4445E+00	1.0913E-04	120.25
633	C16H32	1-CYCLOHEXYLDECANE	-346.683	1.4883E+00	9.8015E-05	106.90
634	C16H34	HEXADECANE	-381.697	1.5241E+00	1.1046E-04	83.68
635	C16H34O	1-HEXADECANOL	-533.675	1.5751E+00	1.1135E-04	-53.01
636	C16H34S	BUTYL-DODECYL-SULFIDE	-322.605	1.4041E+00	2.0806E-04	114.77
637	C16H34S	ETHYL-TETRADECYL-SULFIDE	-321.538	1.4049E+00	2.0836E-04	116.11
638	C16H34S	METHYL-PENTADECYL-SULFIDE	-319.146	1.4075E+00	2.0743E-04	119.20
639	C16H34S	OCTYL-SULFIDE	-322.409	1.4092E+00	2.0873E-04	116.52
640	C16H34S	PROPYL-TRIDECYL-SULFIDE	-321.856	1.4041E+00	2.0804E-04	115.52
641	C16H34S	1-HEXADECANETHIOL	-325.520	1.4048E+00	2.0614E-04	111.88
642	C16H34S2	OCTYL-DISULFIDE	-312.192	1.3851E+00	2.2550E-04	121.08
643	C17H28	1-PHENYLUNDECANE	-165.020	1.2050E+00	9.2372E-05	203.43
644	C17H32	1-HEPTADECYNE	-110.335	1.3802E+00	9.9805E-05	311.04
645	C17H34	1-HEPTADECENE	-276.569	1.4947E+00	1.0958E-04	179.91
646	C17H34	1-CYCLOPENTYLDODECANE	-345.061	1.5413E+00	1.1522E-04	125.94
647	C17H34	1-CYCLOHEXYLUNDECANE	-367.817	1.5854E+00	1.0407E-04	115.31
648	C17H36	HEPTADECANE	-402.745	1.6209E+00	1.1669E-04	92.09
649	C17H36O	1-HEPTADECANOL	-554.820	1.6721E+00	1.1740E-04	-44.64
650	C17H36S	BUTYL-TRIDECYL-SULFIDE	-342.679	1.4965E+00	2.1883E-04	123.22
651	C17H36S	ETHYL-PENTADECYL-SULFIDE	-341.808	1.4980E+00	2.1838E-04	124.47
652	C17H36S	HEXADECYL-METHYL-SULFIDE	-339.362	1.5003E+00	2.1778E-04	127.57
653	C17H36S	PROPYL-TETRADECYL-SULFIDE	-341.939	1.4965E+00	2.1877E-04	123.97
654	C17H36S	1-HEPTADECANETHIOL	-345.747	1.4978E+00	2.1627E-04	120.29
655	C18H30	1-PHENYLDODECANE	-186.163	1.3021E+00	9.8370E-05	211.79
656	C18H30	HEXAETHYLBENZENE	-231.018	1.3613E+00	7.6183E-05	182.46
657	C18H34	1-OCTADECYNE	-131.478	1.4774E+00	1.0574E-04	319.49
658	C18H36	1-OCTADECENE	-297.655	1.5915E+00	1.1579E-04	188.32
659	C18H36	1-CYCOPENTYLTRIDECANE	-363.548	1.6385E+00	1.2095E-04	136.98
660	C18H36	1-CYCLOHEXYLDODECANE	-388.881	1.6821E+00	1.1029E-04	123.72
661	C18H38	OCTADECANE	-423.911	1.7180E+00	1.2257E-04	100.50
662	C18H38O	1-OCTADECANOL	-575.861	1.7690E+00	1.2355E-04	-36.19
663	C18H38S	BUTYL-TETRADECYL-SULFIDE	-362.931	1.5895E+00	2.2894E-04	131.59
664	C18H38S	ETHYL-HEXADECYL-SULFIDE	-361.840	1.5902E+00	2.2925E-04	132.93
665	C18H38S	HEPTADECYL-METHYL-SULFIDE	-359.398	1.5926E+00	2.2863E-04	136.02
666	C18H38S	NONYL-SULFIDE	-362.874	1.5950E+00	2.2922E-04	133.30
667	C18H38S	PENTADECYL-PROPYL-SULFIDE	-362.194	1.5896E+00	2.2887E-04	132.34
668	C18H38S	1-OCTADECANETHIOL	-365.792	1.5899E+00	2.2735E-04	128.74
669	C18H38S2	NONYL-DISULFIDE	-352.424	1.5702E+00	2.4668E-04	137.95
670	C19H32	1-PHENYLTRIDECANE	-207.235	1.3990E+00	1.0443E-04	220.25
671	C19H36	1-NONADECYNE	-152.616	1.5744E+00	1.1175E-04	327.86
672	C19H38	1-NONADECENE	-318.805	1.6887E+00	1.2163E-04	196.73
673	C19H38	1-CYCLOPENTYLTETRADECANE	-384.618	1.7355E+00	1.2721E-04	145.48
674	C19H38	1-CYCLOHEXYLTRIDECANE	-409.956	1.7791E+00	1.1633E-04	132.17
675	C19H40	NONADECANE	-444.994	1.8150E+00	1.2867E-04	108.91
676	C19H40O	1-NONADECANOL	-597.017	1.8661E+00	1.2948E-04	-27.78
677	C19H40S	BUTYL-PENTADECYL-SULFIDE	-380.286	1.6678E+00	2.5645E-04	140.00
678	C19H40S	ETHYL-HEPTADECYL-SULFIDE	-382.174	1.6836E+00	2.3903E-04	141.29
679	C19H40S	HEXADECYL-PROPYL-SULFIDE	-382.299	1.6822E+00	2.3931E-04	140.79
680	C19H40S	METHYL-OCTADECYL-SULFIDE	-379.714	1.6859E+00	2.3849E-04	144.39
681	C19H40S	1-NONADECANETHIOL	-386.116	1.6833E+00	2.3717E-04	137.11
682	C20H34	1-PHENYLTETRADECANE	-228.416	1.4962E+00	1.1037E-04	228.61
683	C20H38	1-EICOSYNE	-173.613	1.6710E+00	1.1807E-04	336.31
684	C20H40	1-EICOSENE	-339.913	1.7856E+00	1.2774E-04	205.14
685	C20H40	1-CYCLOPENTYLPENTADECANE	-405.771	1.8327E+00	1.3312E-04	153.89
686	C20H40	1-CYCLOHEXYLTETRADECANE	-431.135	1.8762E+00	1.2227E-04	140.54
687	C20H42	EICOSANE	-466.086	1.9119E+00	1.3473E-04	117.32
688	C20H42O	1-EICOSANOL	-618.212	1.9633E+00	1.3533E-04	-19.41
689	C20H42S	BUTYL-HEXADECYL-SULFIDE	-403.297	1.7751E+00	2.4959E-04	148.41
690	C20H42S	DECYL-SULFIDE	-403.294	1.7809E+00	2.4954E-04	150.16
691	C20H42S	ETHYL-OCTADECTL-SULFIDE	-402.324	1.7761E+00	2.4974E-04	149.70
692	C20H42S	HEPTADECYL-PROPYL-SULFIDE	-402.579	1.7752E+00	2.4943E-04	149.16
693	C20H42S	METHYL-NONADECYL-SULFIDE	-399.878	1.7786E+00	2.4886E-04	152.80
694	C20H42S	1-EICOSANETHIOL	-406.155	1.7754E+00	2.4814E-04	145.52
695	C20H42S2	DECYL-DISULFIDE	-392.688	1.7552E+00	2.6793E-04	154.77
696	C21H36	1-PHENYLPENTADECANE	-249.518	1.5931E+00	1.1646E-04	237.02
697	C21H42	1-CYCLOPENTYLHEXADECANE	-426.839	1.9296E+00	1.3923E-04	162.30
698	C21H42	1-CYCLOHEXYLPENTADECANE	-452.259	1.9733E+00	1.2822E-04	148.95
699	C22H38	1-PHENYLHEXADECANE	-270.675	1.6903E+00	1.2232E-04	245.43
700	C22H44	1-CYCLOHEXYLHEXADECANE	-473.340	2.0702E+00	1.3439E-04	157.36

NOTE: 1.Temperature range is 298-1000K except for S, Br and I compounds. 2.Temperature range for S, Br and I compounds is 298-717.2K, 332.6-1000K and 458.4-1000K.
3.Additional compounds are: H2O(g) (A=-2.4174E+02, B=4.1740E-02, C=7.4281E-06) AND HCL(g) (A=-9.2209E+01, B=-1.1226E-02, C=2.6966E-06).

8.4 Equilibrium Conversion

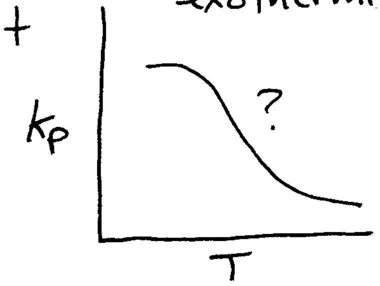
you want highest X_{eq} ← Goal

Van't Hoff equation $\frac{d \ln K_p}{dT} = \frac{\Delta H_{rxn}}{RT^2}$

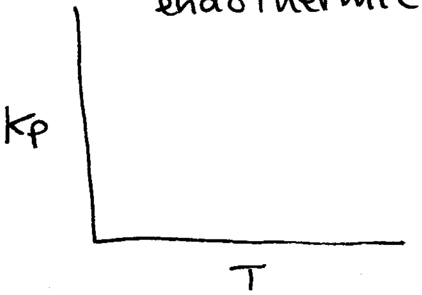
$K_p \equiv \frac{\text{Products}}{\text{Reactants}}$

Plot

exothermic



endothermic

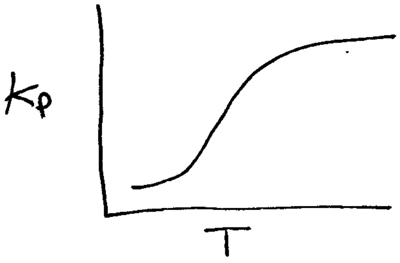


Answer: $\frac{d \ln K_p}{dT}$ is the slope

for exothermic $\Delta H_{rxn} < 0$
so slope is
negative

← at high T's slope = 0

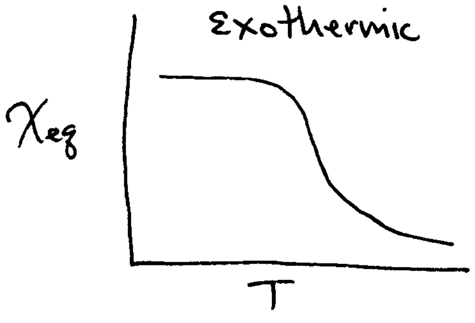
Endothermic $\Delta H_{rxn} > 0$ slope is positive

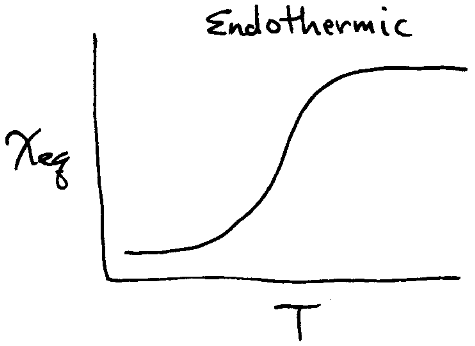


← at high T's slope = 0

Now Relate K_p to X_{eq}

$K_p = \frac{\text{products}}{\text{Reactants}}$ K_p is high X_{eq} is high


Exothermic


Endothermic

OR

Le Chatelier's Principle

$A + B \rightleftharpoons C + D + \text{Heat}$ exothermic

As you add heat the rxn ~~slows down~~ X decreases.

If you remove heat X increases

$A + B + \text{heat} \rightleftharpoons C + D$ ENDOTHERMIC

If you add heat you get a higher X

11/5/91-1

(Sandler Thermo

$k = A\exp\left[\frac{\text{[illegible]}}{RT}\right]$?

8.4 Equilibrium Conversion

For Endothermic "X_{eq}" is the equilibrium "max" with Reversible Reactions

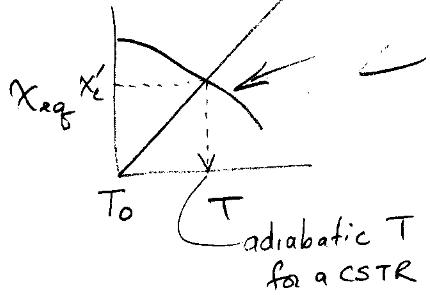
$$r = k\left(C_A C_B - \frac{C_D C_C}{K_{eq}}\right)$$

Exothermic X_{eq} ↓ with T ↑

Energy Balance $\frac{\Sigma \Theta C_{p_i}}{-\Delta H_{Rxn}}$ slope

8.4.1 $\varphi = 0$

Exothermic



rxn rate

$$r = 0 = k_f\left(C_A C_B - \frac{C_C C_D}{K}\right)$$

k_f: f(T)

K: ∴ f(T)

$$K \equiv \frac{k_f}{k_{rev}}$$

Energy Balance solving for X

$$X = \frac{\Sigma \Theta_i \tilde{C}_{p_i}(T - T_0)}{-\underbrace{\left[\Delta H^\circ_{rxn}\Big|_{T_R} + \Delta\tilde{C}_p(T - T_R)\right]}_{-\Delta H_{Rxn}|_T}}$$

from $\underline{\underline{8\text{-}41}}$

② $K_p = K_c(RT)^\delta$

① $K_p = \frac{P_C^{c/a} P_D^{d/a}}{P_A P_B^{b/a}}$

③ van't Hoff Relation $\frac{d \ln K_p}{dT} = \frac{\Delta H_{rxn}|_T}{RT^2}$

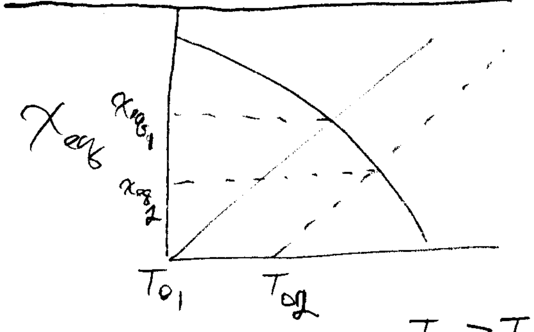
see aside on PFR

$$X = \left(\frac{\Sigma \Theta_i \tilde{C}_{p_i}}{-\Delta H_{Rxn}}\right)(T - T_0)$$

if ΔH_{rxn} does not vary in the temperature range $(T - T_0)$!

not stated in book

Look at Exothermic Rxns



What happens if T_o increases 8.4.2

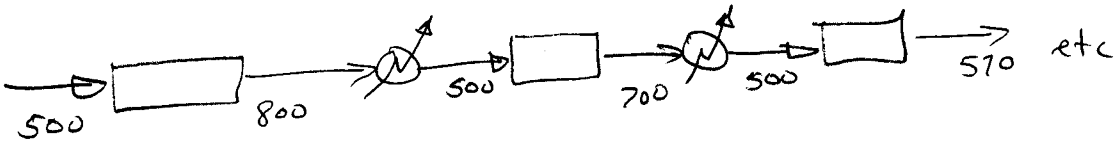
$T_{o_2} > T_{o_1}$ (Increase entering fluid Temp)

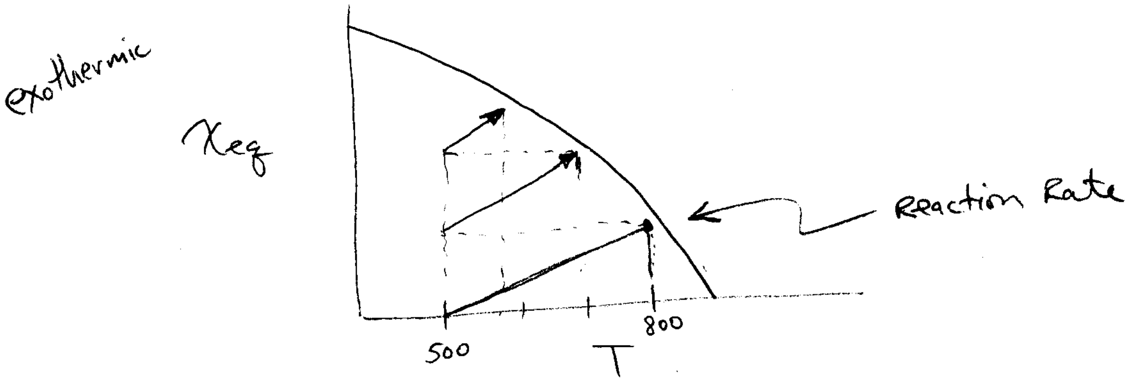
$X_{eq_2} < X_{eq_1}$

11/5/91 - 2

Interstage Cooling

Higher conversions





Endothermic

Interstage heating

$430 < T < 530$

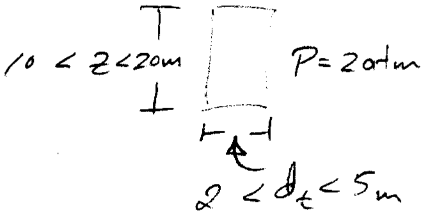
NO Rxn — side Rxn

upgrading crude oil

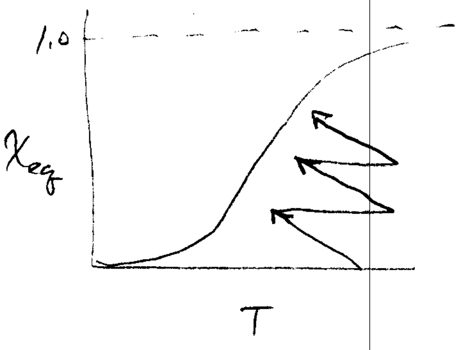
dehydrogenation

straight chain Alkanes → ARomatics

Endo



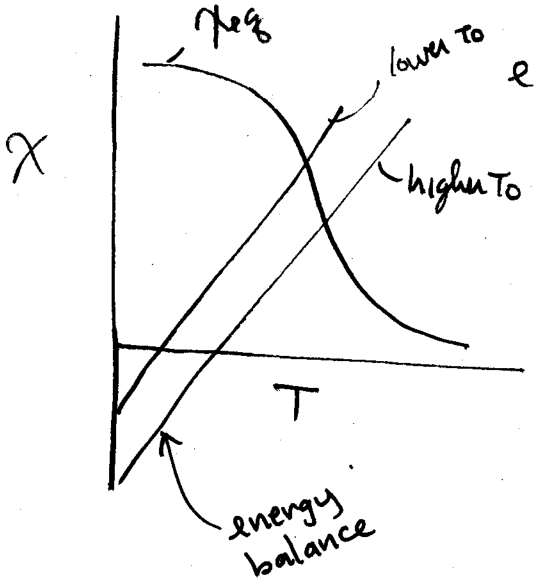
{ 1million $ of Catalyst! per Reactor }



8.5.2
~~8.4.2~~ optimum feed Temperature

Discuss :

Approximate methods for adiabatic reactors equilibrium limited.



exothermic

$\Delta H_{rxn} < 0$

But lowering the To also lowers the rate of reaction

$$X = \frac{\sum \frac{F_{i0}}{F_{A0}} \tilde{C}_{p_i} (T - T_0)}{-\Delta H_{rxn}}$$

$$= T \left(\frac{\frac{\sum F_{i0} C_{p_i}}{F_{A0}}}{-\Delta H_{rxn}} \right) + \left(\frac{\frac{\sum F_{i0} C_{p_i}}{F_{A0}}}{\Delta H_{rxn}} \right) T_0$$

To small then intercept is a small negative number

if To large Intercept large Negative number

Unsteady-state & multiple steady-states
8.6

Read 8.5 $SO_2 + \frac{1}{2}O_2 \xrightarrow{V_2O_5} SO_3$

$$\rho_b = \left(33.8\ \mathrm{lbm/ft^3}\right)\left(\frac{0.4535\ \mathrm{kg}}{\mathrm{lbm}}\right)\left(\frac{\mathrm{ft}}{0.3048\ \mathrm{m}}\right)^3$$
$$= 541.9\ \mathrm{kg/m^3}$$

Example of interstage cooling

8.6 Multiple Steady-states

Objective: predict the stable operation of a CSTR

~~8.6.3~~

8.7 Nonisothermal Multiple Rxns

presented before

8.5 - 8.7

Unsteady-state and multiple steady-states

Multiple steady-states - 8.7

CSTR :

$$V \sum_{i=1}^{n} C_{p_i} C_i \cancel{\frac{dT}{dt}} = UA(T_a - T) - \dot{W}_s - F_{A0} \sum_{i=1}^{n} \frac{F_{i0}}{F_{A0}} \tilde{C}_{p_i} (T - T_0) - \Delta H_R\big|_T (-r_A V)$$

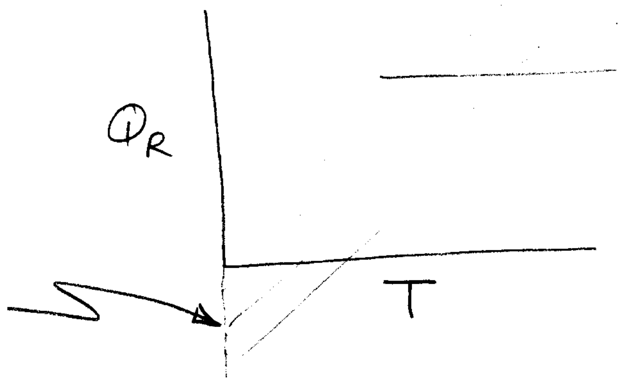
0

Steady state $$\frac{d(C_i V)}{dt} = F_{A0} - F_A + r_A V$$

Set $\dot{W}_s = 0$ $\quad F_{A0} X_A = F_{A0} - F_A$ By definition

$$\underbrace{UA(T - T_a) + \sum_{i=1}^{n} F_{i0} \tilde{C}_{p_i} (T - T_0)}_{\text{Heat "Removed" } Q_R} = \underbrace{\Delta H_R (r_A V)}_{\text{Heat generated } Q_{gen}}$$

$$T \underbrace{\left[UA + \sum_{i=1}^{n} F_{i0} \tilde{C}_{p_i} \right]}_{\text{slope}} - \underbrace{T_a UA - \sum_{i=1}^{n} F_{i0} C_{p_i} T_0}_{\text{intercept}} = \Delta H_R (r_A V)$$

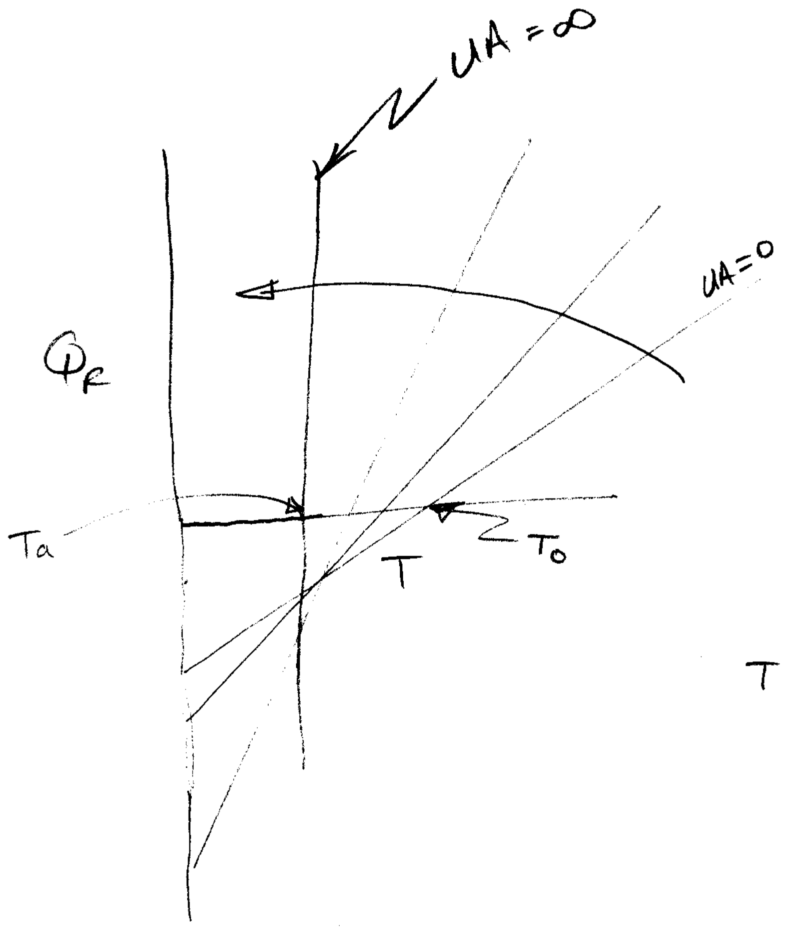


Intercept is negative

→ Increasing T_0 (a inlet temperature)

Increasing T_a

~~Increasing UA~~ (But slope increases as well)



for $T_a < T_0$

(T_a is used for cooling)

Increasing UA

Changes slope and intercept

Note $Q_R = 0$

$$T = \frac{\left(\Sigma F_{i0} C_{p_i}\right) T_0 + UA\, T_a}{\Sigma F_{i0} C_{p_i} + UA}$$

at $UA = 0$

$T = T_0$

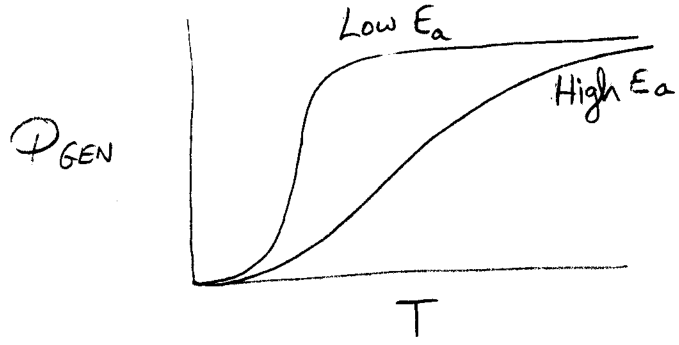
at $UA >> \Sigma F_{i0} C_{p_i}$ $(UA = \infty)$

$T = T_a$

Heat generation:

$$\Delta H_{Rxn}\, r_A V = \Delta H_{Rxn}\left(-k\, f(c)\right) V$$

$$A \exp\left(-\frac{E}{RT}\right)$$



$$\frac{A}{\exp(E/RT)}$$

$T \to \infty$

$A/\exp(E/RT) \to A$

$T \to$ small

$A/\exp(E/RT) \to 0$

$$\exp\left(-\frac{E_{High}}{RT}\right) \text{ vs } \exp\left(-\frac{E_{Low}}{RT}\right)$$

$\frac{1}{e}$ $\quad$ $1/\exp\left(+\frac{1000}{T}\right)$ $\quad$ $1/\underbrace{\exp\left(+\frac{1}{T}\right)}$

increases the change $\quad$ delays the change

8.~~6~~7.4 Runaway Reactions

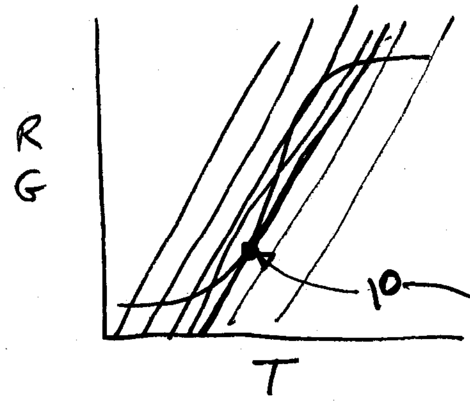


Fig 8-23

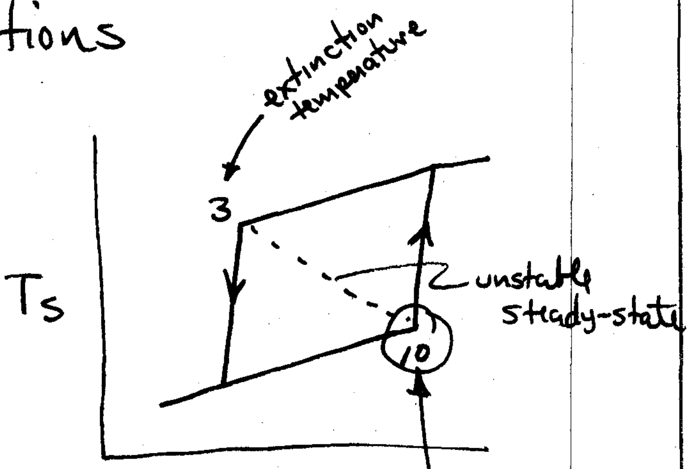


Fig 8-24

Ignition temperature giving a jump in rxn Temp

equation ~~8-77~~ 8-71 $\frac{dG}{dT} = \frac{dR}{dT}$ equal slopes

$-dr/dT = E/RT^2(-r_A)$

$\Delta T_{rc} = T_r - T_c = \frac{R T_r^2}{E}$ } Back of the envelope

T_c given by 8-66 page 491 (a mess) $= \frac{T_0 F_{A0} C_{p0} + UAT_0}{UA + C_{p0} F_{A0}}$

T_r = CSTR reactor temperature

if the reactor temperature rises to $\underline{\underline{10}}$ then runaway occurs or if $T_r - T_c > \Delta T_{rc}$ then runaway occurs.

$\cancel{C_{P_0}(1+k)}(T-T_c) = \underline{-\cancel{r_A V/F_{A0}} - \Delta H_{Rxn}}$ ← 8-67

$C_{P_0} \cancel{(1+k)} = \frac{E}{RT^2}(\cancel{-r_A}) \frac{-\Delta H_{Rxn}}{F_{A0}} \cancel{V}$ ← 8-76

$T - T_c = \frac{RT^2}{E}$

$16 < \frac{E}{RT} < 24$

$300 < T < 500K$

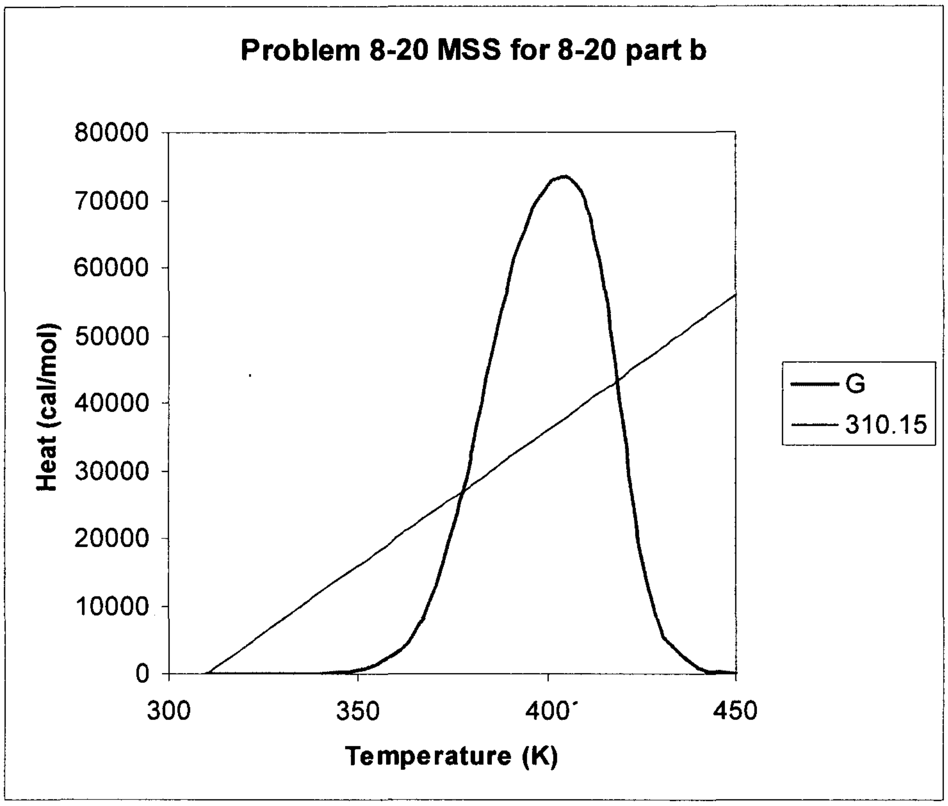
$\Delta T \sim \underline{\underline{15 \text{ to } 30°C}}$

Steady - state CSTR

$A \rightleftharpoons B$ liquid phase

Problem ~~8-8b~~ 8-20

The steady-state temperatures are



On the Spreadsheet the values can be found by trial and error or the solver to give

Steady state Temps

Part b) T= 310.2, 377.5, and 418.4 K

Part c) T= 310.2 and 418.4 K are stable and 377.5 K is unstable.

Part d) the conversion corresponding to T= 418.4 K is $\chi_A = 0.54$

$$UA(T_a - T) - F_{A0}C_{P_A}(T - T_0) = \Delta H_{rxn} F_{A0} \underset{\uparrow}{X_A}$$

Plug in m.B. solution

8-20 e)

Determine MSS

$T_0 = 310.15k$

	$T_A(k)$	T_L	T_m	T_H	
T_{a_1}	175	188.5	–	–	— 1 soln
T_{a_2}	208	218.2	190	–	← 2 soln
T_{a_3}	250	256	387	413	3 soln
T_{a_4}	310.15	310.2	377.5	418.4	
T_{a_5}	350	347	367.5	421.4	
T_{a_6}	357	357.2	361.2	421.9	
T_{A_6}'			361	422	← 2 solns
T_{a_7}	400	–	–	426	← 1 soln
~~T_{a_8}~~	~~210~~	~~220.0~~	~~399.7~~	~~403.8~~	
T_{a_8}	410			430?	

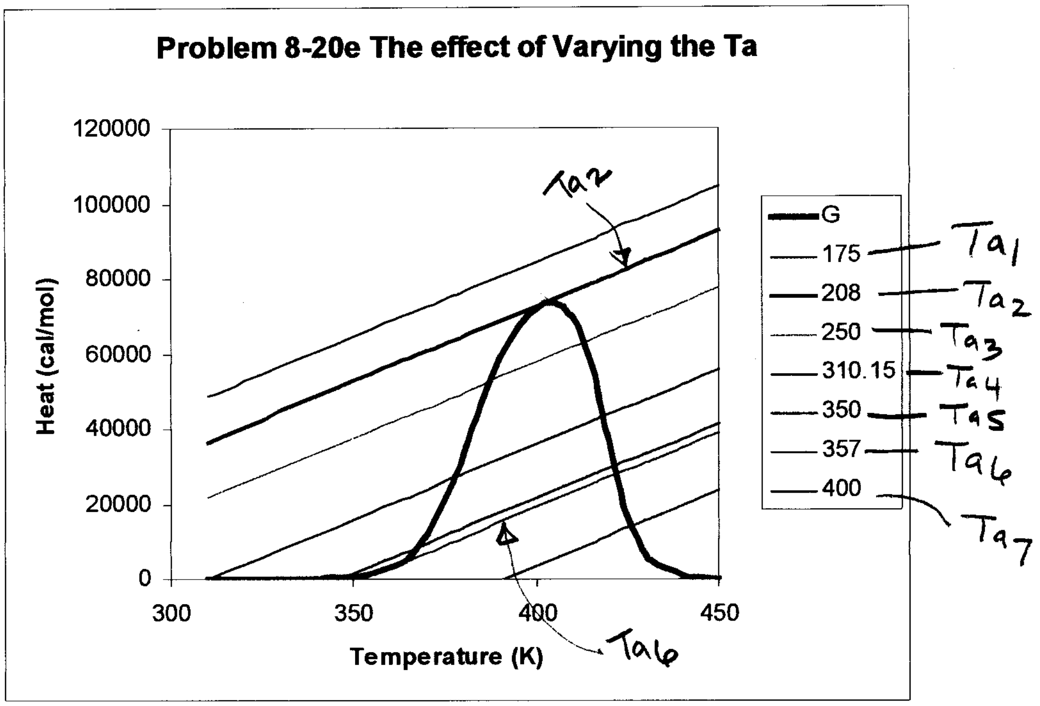
for UA = 0

$$T_L \quad \underbrace{310 \qquad 431}_{\text{stable}} \qquad \underset{\text{unstable}}{357k}$$

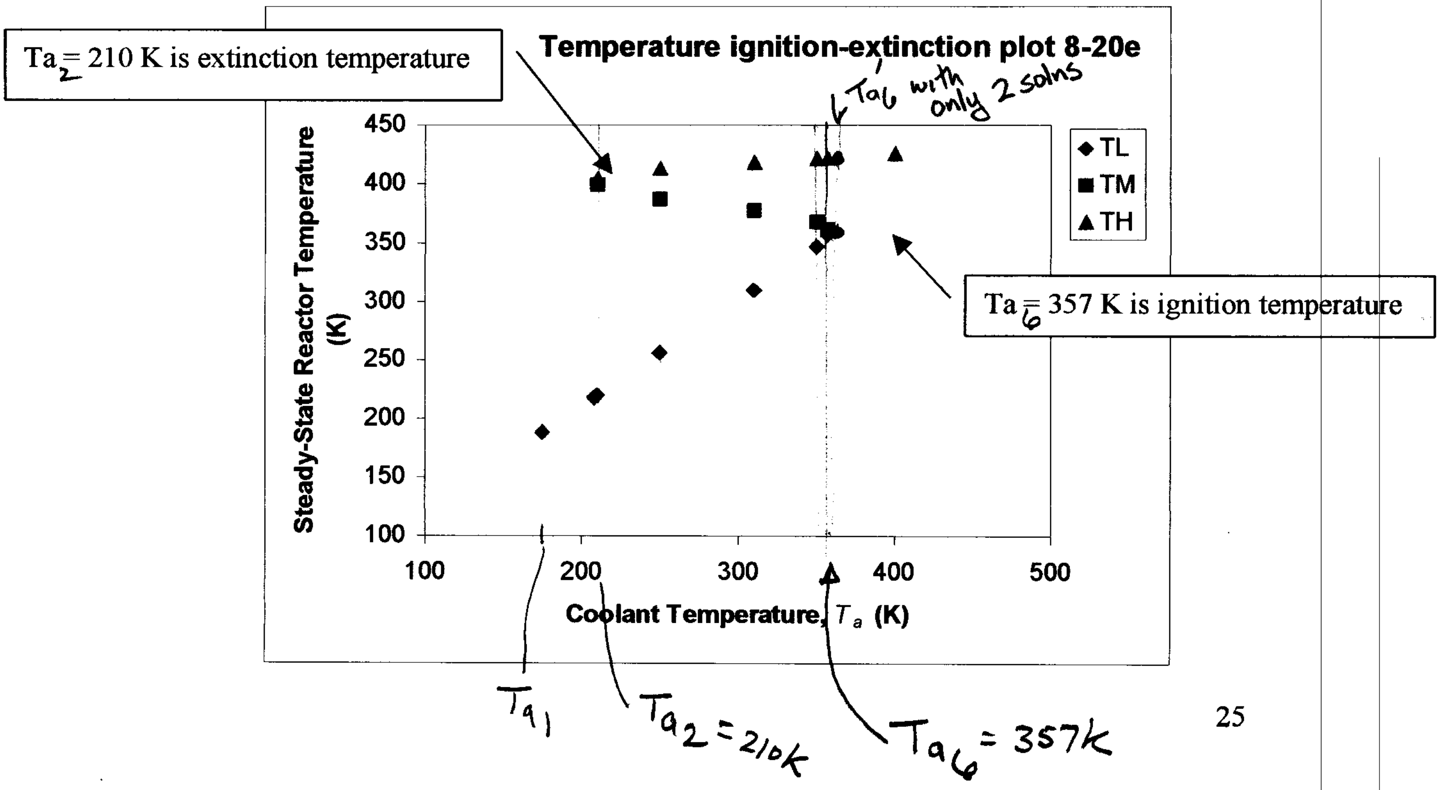
at T = 431

$X_A = 0.061$ ← this is an equilibrium conversion

Problem 8-20 part e



In these simulations the lines for the heat removal term R are parallel. The ignition and the extinction temperatures are are determined from the analysis which will either blow out the temperature or ignite the reactor temperature.



Design Project

Thursday:

Bring c_p's, ΔH^f } for each component

Calc. ΔH_{rxn} for each reaction

start with using average C_p values.

(this may be all you need) – you will need to justify this from a hand or spreadsheet calculation

[redacted]

Design Project: Polymath

$$\frac{dT}{dV} = \frac{Ua(Ta-T) + \sum_{i=1}^{q} (+r_{ij})(\Delta H_{rxn\,ij})}{\sum_{j=1}^{m} F_j \, c_{p_j}}$$

8-76 page 544

m # of j components

q # of i rxns

[redacted]

End of class we will have a working energy balance.