Example 9.3.3/ Problem #3

Here is the rate constant. Note that in Mathematica, “=” assigns the symbol on the left to the expression on the right, (basically giving an expression a nickname.)

```
In[∘]:= kT = 5 × 10^-3 Exp[20000 / 8.314 (1 / 300 - 1 / T[t])]
```

$$\text{Out[∘]=}\ \frac{1}{200}\, e^{2405.58 \times \left(\frac{1}{300} - \frac{1}{T[t]}\right)}$$

Here is the mass balance for component “A”

```
In[∘]:= faeq = kT .5 (1 - fa[t]) (1.2 - fa[t])
```

$$\text{Out[∘]=}\ 0.0025\, e^{2405.58 \times \left(\frac{1}{300} - \frac{1}{T[t]}\right)} (1 - fa[t]) \times (1.2 - fa[t])$$

Here is the energy balance for the book example

```
In[∘]:= Teqad = (50 (300 - T[t]) - (-15000) × (100) kT .5 (1 - fa[t]) (1.2 - fa[t])) /
          (100 (1 - fa[t]) 65 + 100 (1.2 - fa[t]) 65 + 100 fa[t] 150)
```

$$\text{Out[∘]=}\ \frac{3750.\, e^{2405.58 \times \left(\frac{1}{300} - \frac{1}{T[t]}\right)} (1 - fa[t]) \times (1.2 - fa[t]) + 50 \times (300 - T[t])}{6500 \times (1 - fa[t]) + 6500 \times (1.2 - fa[t]) + 15000\, fa[t]}$$

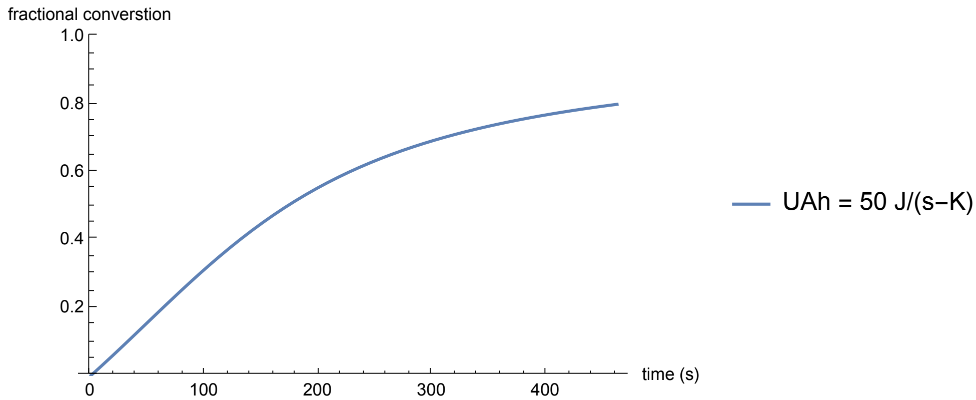
```
In[∘]:= answer = NDSolve[{D[fa[t], t] == faeq, D[T[t], t] == Teqad,
           fa[0] == 0, T[0] == 300}, {fa[t], T[t]}, {t, 0, 550}]

Out[∘]= {{fa[t] → InterpolatingFunction[ Domain: {{0., 550.}} Output: scalar ][t],
          T[t] → InterpolatingFunction[ Domain: {{0., 550.}} Output: scalar ][t]}}
```

```
In[∘]:= (fa[t] /. answer[[1]]) /. t → 462

Out[∘]= 0.799805
```

```
In[∘]:= (T[t] /. answer[[1]]) /. t → 462

Out[∘]= 331.623
```

```
In[∘]:= Plot[fa[t] /. answer[[1]], {t, 0, 462}, PlotRange → {0, 1},
         AxesLabel → {"time (s)", "fractional converstion"},
         PlotLegends → {"UAh = 50 J/(s-K)"}]
```

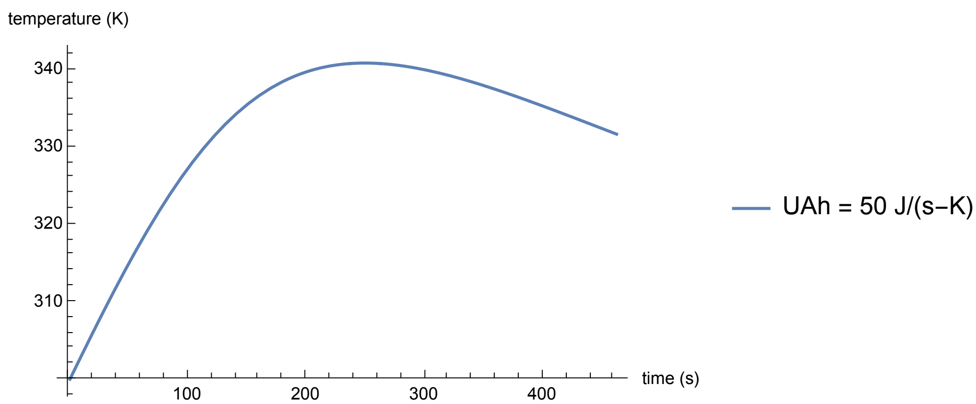
Out[∘]=



In[∘]:=

```
Plot[T[t] /. answer⟦1⟧, {t, 0, 462},
 AxesLabel → {"time (s)", "temperature (K)"}, PlotLegends → {"UAh = 50 J/(s-K)"}]
```

Out[∘]=



Here is the heat removal rate:

In[∘]:=

```
NIntegrate[ 50 ( 300 - T[t] /. answer⟦1⟧), {t, 0, 462}]
```

Out[∘]= -741582.

In[∘]:=

```
100 × .7925 × 15000
```

Out[∘]= 1.18875×10^6

Change in enthalpy for products-reactants

In[∘]:=

```
100 ( (1 - .7925) × 65 + (1.2 - .7925) × 65 + .7925 × 200) 331.71 -
 100 ( 1 × 65 + 1.2 × 65 + 0 × 130) 300
```

Out[∘]= 2.29361×10^6

In[∘]:=

```
% - %%
```

Out[∘]= 1.10486×10^6

In[∘]:=

```
100 ( (1 - .7998) × 65 + (1.2 - .7998) × 65 + .7998 × 130) 31.623
```

Out[∘]= 452209.

Here is the energy balance for the homework problem. UA = 0

In[∘]:=
```
Teqad = (0 (300 - T[t]) - (-15 000) × (100) kT .5 (1 - fa[t]) (1.2 - fa[t])) /
  (100 (1 - fa[t]) 65 + 100 (1.2 - fa[t]) 65 + 100 fa[t] 150)
```

Out[∘]=
$$\frac{3750.\ e^{2405.58\times\left(\frac{1}{300}-\frac{1}{T[t]}\right)}\ (1-fa[t])\times(1.2-fa[t])}{6500\times(1-fa[t])+6500\times(1.2-fa[t])+15000\ fa[t]}$$

In[∘]:=
```
hwanswer = NDSolve[{D[fa[t], t] == faeq, D[T[t], t] == Teqad,
   fa[0] == 0, T[0] == 300}, {fa[t], T[t]}, {t, 0, 500}]
```

Out[∘]=
```
{{fa[t] → InterpolatingFunction[ Domain: {{0., 500.}} Output: scalar ][t],
  T[t] → InterpolatingFunction[ Domain: {{0., 500.}} Output: scalar ][t]}}
```

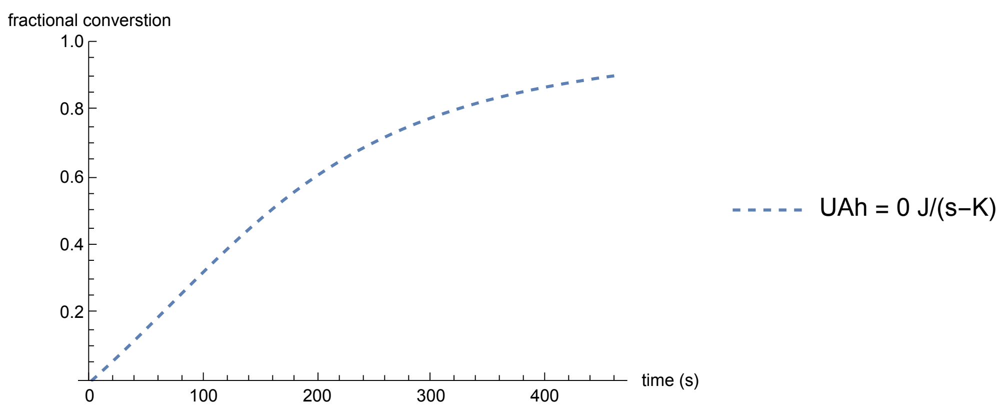
In[∘]:=
```
(fa[t] /. hwanswer[[1]]) /. t → 462
```

Out[∘]= 0.902252

In[∘]:=
```
(T[t] /. hwanswer[[1]]) /. t → 462
```

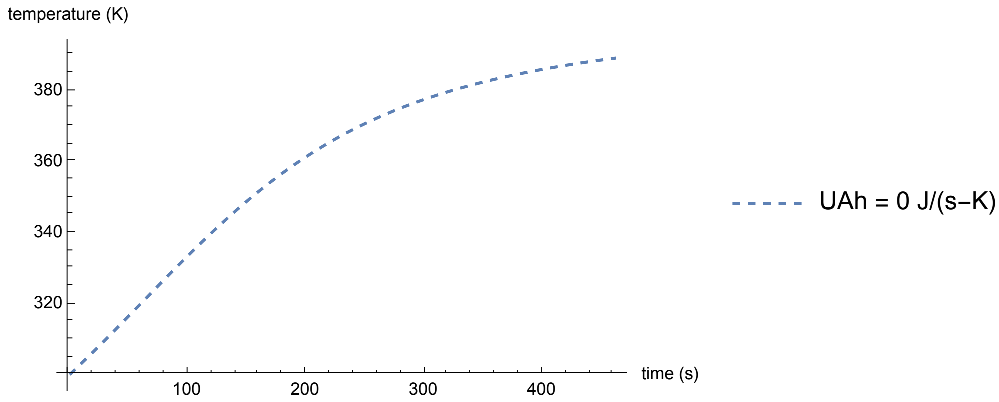
Out[∘]= 389.13

In[∘]:=
```
Plot[fa[t] /. hwanswer[[1]], {t, 0, 462}, PlotRange → {0, 1},
 AxesLabel → {"time (s)", "fractional converstion"},
 PlotLegends → {"UAh = 0 J/(s-K)"}, PlotStyle → Dashed]
```

Out[∘]=


In[∘]:=
```
Plot[T[t] /. hwanswer[[1]], {t, 0, 462},
 AxesLabel → {"time (s)", "temperature (K)"},
 PlotLegends → {"UAh = 0 J/(s-K)"}, PlotStyle → Dashed]
```

Out[∘]=

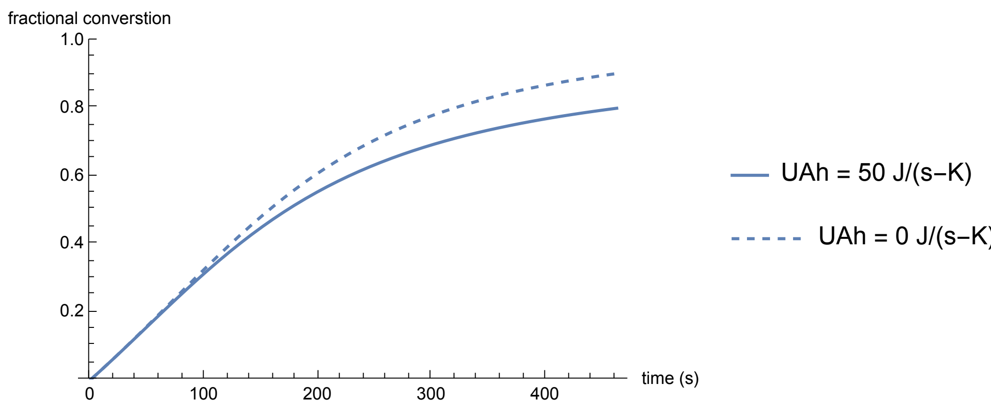


Compare answers:

In[∘]:=

```
Show[%351, %360]
```

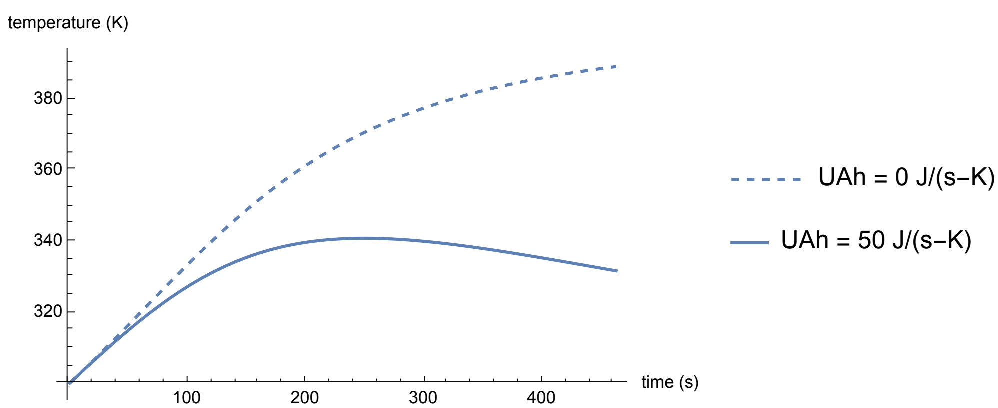
Out[∘]=



In[∘]:=

```
Show[%362, %352]
```

Out[∘]=



Heat removed for example 9.3.3

Looking at the Q-dot term, the heat removal rate integrated for the time is. This is in Joules.

In[∘]:=

```
NIntegrate[ 50 (T[t] - 300) /. answer[[1]], {t, 0, 462}]
```

Out[∘]= 741 582.

Problem 7

Here are the original equations:

In[∘]:=
```
massbalanceeq = - 4 y[x] Exp[ 18 ( 1 - 1 / θ[x])]
```

Out[∘]= $-4\, e^{18\times\left(1-\frac{1}{\theta[x]}\right)}\, y[x]$

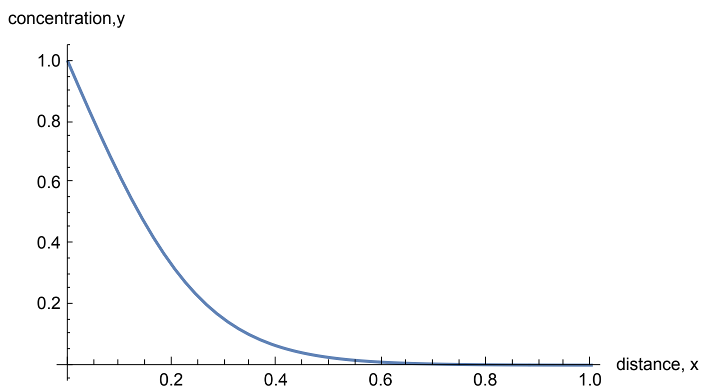
In[∘]:=
```
energybalanceeq =  .2 y[x] Exp[ 18 ( 1 - 1 / θ[x])]
```

Out[∘]= $0.2\, e^{18\times\left(1-\frac{1}{\theta[x]}\right)}\, y[x]$

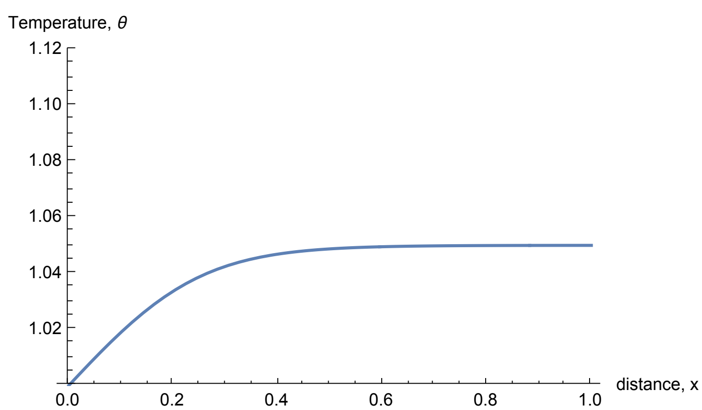
In[∘]:=
```
ans3 = NDSolve[{ D[y[x], x]  == massbalanceeq,
   D[θ[x], x]  == energybalanceeq, θ[0]  == 1, y[0]  == 1}, {y[x], θ[x]}, {x, 0, 1}]
```

Out[∘]=
```
{{y[x] → InterpolatingFunction[ Domain: {{0., 1.}} Output: scalar ][x],
  θ[x] → InterpolatingFunction[ Domain: {{0., 1.}} Output: scalar ][x]}}
```

In[∘]:=
```
cans1 =
 Plot[y[x] /. ans3[[1]], {x, 0, 1}, AxesLabel → {"distance,  x", "concentration,y"}]
```

Out[∘]=


In[∘]:=
```
Plot[θ[x] /. ans3[[1]], {x, 0, 1},
 AxesLabel → {"distance,  x", "Temperature,  θ"}, PlotRange → {1, 1.12}]
```

Out[∘]=


Redo with the heat reaction term doubled

In[∘]:=
```
massbalanceeq = - 4 y[x] Exp[ 18 (1 - 1 / θ[x])]
```

Out[∘]= $-4\, e^{18\times\left(1-\frac{1}{\theta[x]}\right)}\, y[x]$

In[∘]:=
```
doubleenergybalanceeq =  .4 y[x] Exp[ 18 (1 - 1 / θ[x])]
```

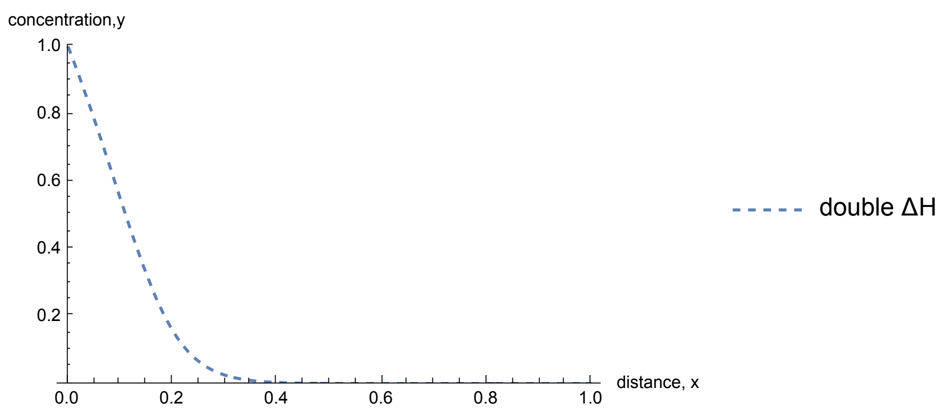
Out[∘]= $0.4\, e^{18\times\left(1-\frac{1}{\theta[x]}\right)}\, y[x]$

In[∘]:=
```
ans3dbl = NDSolve[{ D[y[x], x] == massbalanceeq,
   D[θ[x], x] == doubleenergybalanceeq, θ[0] == 1, y[0] == 1}, {y[x], θ[x]}, {x, 0, 1}]
```

Out[∘]=
```
{{y[x] → InterpolatingFunction[ Domain: {{0., 1.}} Output: scalar ][x],
  θ[x] → InterpolatingFunction[ Domain: {{0., 1.}} Output: scalar ][x]}}
```

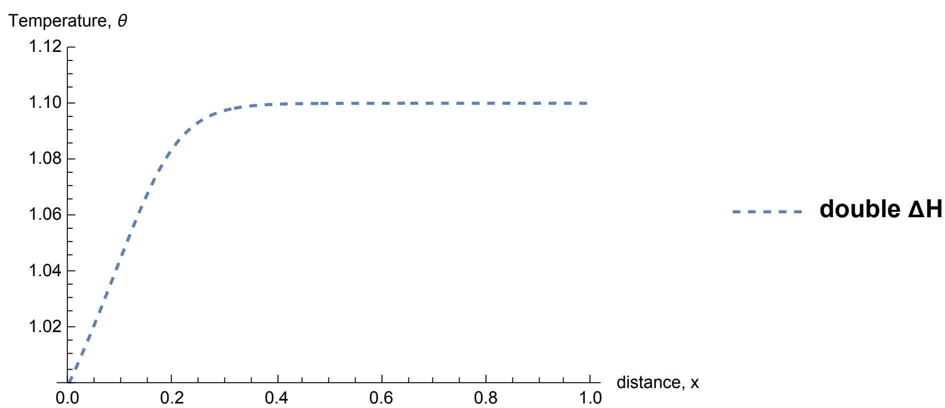
In[∘]:=
```
cans1db =
 Plot[y[x] /. ans3dbl[[1]], {x, 0, 1}, AxesLabel → {"distance, x", "concentration,y"},
  PlotStyle → Dashed, PlotLegends → {"double ΔH"}, PlotRange → {0, 1}]
```

Out[∘]=

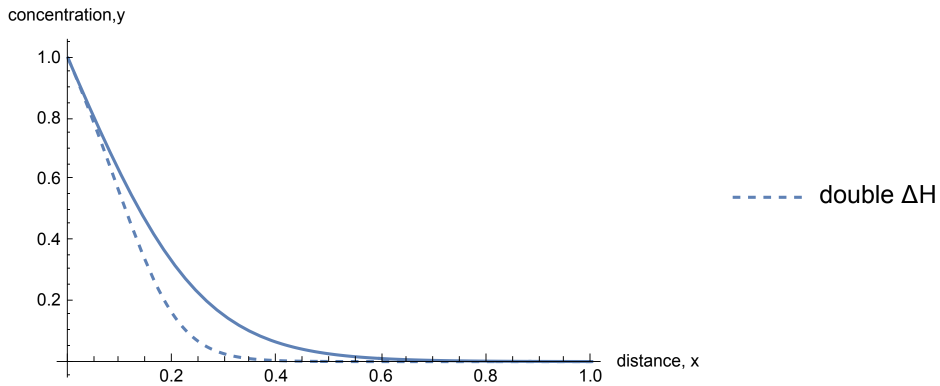


In[∘]:=
```
Plot[θ[x] /. ans3dbl[[1]], {x, 0, 1},
 AxesLabel → {"distance, x", "Temperature, θ"}, PlotRange → {1, 1.12},
 PlotStyle → Dashed, PlotLegends → {"double ΔH"}, PlotRange → {0, 1}]
```

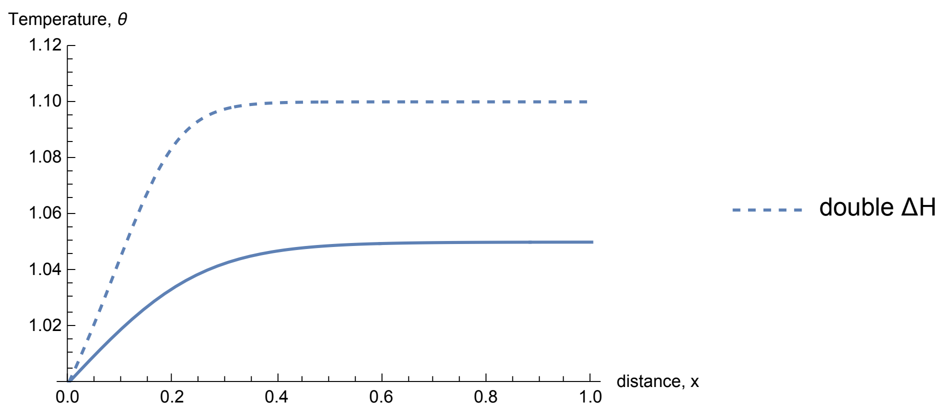
In[∘]:=



In[∘]:= `Show[%374, %381]`

Out[∘]=


In[∘]:= `Show[%375, %383]`

Out[∘]=


Problem #9

Mass balance, e + b-> M

In[∘]:= `eq1 = 0 == qef cef - q ce - k ce cb V`

Out[∘]= `0 == -ce q + cef qef - cb ce k V`

In[∘]:= `eq2 = 0 == qbf cbf - q cb - k ce cb V`

Out[∘]= `0 == -cb q + cbf qbf - cb ce k V`

In[∘]:= `eq3 = q == qef + qbf`

Out[∘]= `q == qbf + qef`

In[∘]:= `ans9 = Solve[{eq1, eq2, eq3}, {ce, cb, q}]`

In[∘]:=
```
ans9 /. {cef → 1, qef → 20, cbf → 4,
   qbf → 10, V → 6500, k → 10^14 Exp[(-11000. / 303)]}
```

Out[∘]= `{{ce → 0.163427, cb → 0.830093, q → 30}, {ce → -1.09966, cb → -0.432998, q → 30}}`

part a

We like the first set of answers best.

The conversion is moles is 1- (moles e exiting/(moles e in feed)

```
In[∘]:= 1 - q ce / (qef cef)
```

$$\text{Out}[\circ]= 1 - \frac{\text{ce q}}{\text{cef qef}}$$

```
In[∘]:= (%393 /. ans9[[1]]) /.
  {cef → 1, qef → 20, cbf → 4, qbf → 10, V → 6500, k → 10^14 Exp[(-11000. / 303)]}
Out[∘]= 0.75486
```

heat removal rate = heat production rate

heat production = ΔH* k ce cb V

the reaction rate is: (mol/s)

part b

```
In[∘]:= 10^14 Exp[(-11000. / 303)] 0.16342 × 0.8300
Out[∘]= 0.00232229
```

The rate of heat removal: (cal/s)

```
In[∘]:= -45000 × 10^14 Exp[(-11000. / 303)] 0.16342 × 0.8300 × 6500
Out[∘]= -679271.
```

The required area is: (m/s)

```
In[∘]:= 679271 / (15000 (30 - 18.))
Out[∘]= 3.77373
```

part c

Without cooling, the temperature will be higher and hence the rate will be faster and the conversion more than .755. We could iterate with the temperature and rate and get an answer. However we could get a pretty good answer if we just pick the conversion as 1.

In this case the moles reacted per time is qef cef.

The energy balance is hence

```
In[∘]:= ΔH * qef cef + q cp (T - 30)
Out[∘]= cp q (-30 + T) + cef qef ΔH
```

```
In[•]:= Solve[% == 0, T]
```

$$\left\{\left\{T \to \frac{30\ cp\ q - cef\ qef\ \triangle H}{cp\ q}\right\}\right\}$$

```
In[•]:= %400 /. { cef → 1., qef → 20, ΔH → - 45 000, cp →  1000, q → 30 }
Out[•]= {{T → 60.}}
```

Or if we want a better answer

```
In[•]:= eq11 = eq1 /. k → 10^14 Exp[(-11 000. / T)]
```

$$0 == -ce\ q + cef\ qef - 100\,000\,000\,000\,000\ cb\ ce\ e^{-11\,000./T}\ V$$

```
In[•]:= eq21 = eq2 /. k → 10^14 Exp[(-11 000. / T)]
```

$$0 == -cb\ q + cbf\ qbf - 100\,000\,000\,000\,000\ cb\ ce\ e^{-11\,000./T}\ V$$

```
In[•]:= ebalance  = ΔH k ce cb V + q cp (T - 303)
```

$$cp\ q\ (-303 + T) + cb\ ce\ k\ V\ \triangle H$$

```
In[•]:= ebalance1 = ebalance /. k → 10^14 Exp[(-11 000. / T)]
```

$$cp\ q\ (-303 + T) + 100\,000\,000\,000\,000\ cb\ ce\ e^{-11\,000./T}\ V\ \triangle H$$

```
In[•]:= eqs = {eq11 , eq21, ebalance1 == 0}
```

$$\{0 == -ce\ q + cef\ qef - 100\,000\,000\,000\,000\ cb\ ce\ e^{-11\,000./T}\ V,$$
$$0 == -cb\ q + cbf\ qbf - 100\,000\,000\,000\,000\ cb\ ce\ e^{-11\,000./T}\ V,$$
$$cp\ q\ (-303 + T) + 100\,000\,000\,000\,000\ cb\ ce\ e^{-11\,000./T}\ V\ \triangle H == 0\}$$

```
In[•]:= eqs /. {cef → 1.`, qef → 20, ΔH → -45 000, cp → 1000, V → 6500, q → 30, cbf → 4, qbf → 10}
```

$$\{0 == 20. - 30\ ce - 650\,000\,000\,000\,000\,000\ cb\ ce\ e^{-11\,000./T},$$
$$0 == 40 - 30\ cb - 650\,000\,000\,000\,000\,000\ cb\ ce\ e^{-11\,000./T},$$
$$-29\,250\,000\,000\,000\,000\,000\,000\ cb\ ce\ e^{-11\,000./T} + 30\,000 \times (-303 + T) == 0\}$$

```
In[•]:= FindRoot[eqs /. { cef → 1., qef → 20, ΔH → - 45 000, cp →  1000,
           V → 6500, q → 30,  cbf →  4, qbf →  10 }, { ce, .01}, {cb, .4}, {T, 350}]
Out[•]= {ce → 0.010397, cb → 0.677064, T → 332.532}
```

So the real temperature is

```
In[•]:= 332.5 - 273.4
Out[•]= 59.1
```

Which is not significantly different from the simpler answer.

```
import numpy as np
import matplotlib.pyplot as plt
from scipy.integrate import odeint
```

Problem 10.10

Liquid-phase reaction $A \to B$ is to be carried out in a tubular reactor operating at 202.6 kPa. The feed rate is 600 kmol/ks of pure A at 200 $^\circ$C. Pure A has a specic volume of 0.056 $m^3/kmol$. The heat of reaction at this T is -15 kJ/mol. The molar specific heats of A and B and both 42 J/(mol K). The reaction rate constant can be approximated by

$$k = 110 + 0.8(T - 200)$$

for k in 1/ks and T in $^\circ$C. The maximum reaction temperature allowable is 400 $^\circ$C. Calculate the minimum reactor volume required to obtain 80% conversion of A. What must the heat transfer rate be in the cooled section of the reactor? Reactor diameter is 5 cm.

In the adiabatic section,

```
H_rxn = -15 * 1000 # J/mol
T0 = 200 # C
Tf = 400 # C
FA0 = 600 # mol/s
CA0 = 1/0.056 * 1000 # mol/m^3
V0 = FA0/CA0
Cp_A = 42
Cp_B = 42

def k_func(T):
    return (110 + 0.8*(T - 200))/1000 # in 1/s

def adiabatic_section(TX,V):
    T,X = TX

    k = k_func(T)
    CA = CA0 * (1-X)
    CB = CA0 * X
    r = k * CA
    dTdV = (-H_rxn*r)/(V0*CA*Cp_A + V0*CB*Cp_B)
    dXdV = r/FA0
    return dTdV,dXdV

volume_space = np.linspace(0,1.0,10000)
```

```
initial_cond = [T0,0]

# Numerical integration over volume
adiabat_soln = odeint(adiabatic_section,initial_cond,volume_space)
T_soln = adiabat_soln[:,0]
X_soln = adiabat_soln[:,1]

# Find the index where T is closest to 400 C
print(np.argmin(np.abs(T_soln-400)))
end_idx_ad = np.argmin(np.abs(T_soln-400))
print(T_soln[end_idx])
print('Conversion at end of adibatic section:',round(X_soln[end_idx_ad],3))
print('Volume of adibatic section:', round(volume_space[end_idx_ad],3), 'm^3')
```

```
1459
555.6131460528696
Conversion at end of adibatic section: 0.56
Volume of adibatic section: 0.146 m^3
```

From a mass balance

$$\frac{dV}{dX} = \frac{F_{A,0}}{-\nu_A r}$$

Integrate from conversion at end of adiabatic section (0.56) to desired (0.8) to solve for volume of isothermal section

```
def isothermal_section(V,X):
    k = k_func(400)

    dVdX = FA0/(k*CA0*(1-X))
    return dVdX

initial_cond_isotherm = [0]
conv_space = np.linspace(0.56,0.98,10000)

# Numerical integration over conversion
isotherm_soln = odeint(isothermal_section,initial_cond_isotherm,conv_space)
vol_soln = isotherm_soln[:,0]

# Find index where conversion is closest to 0.8
print(np.argmin(np.abs(conv_space-0.8)))
end_idx_iso = np.argmin(np.abs(conv_space-0.8))
print('Conversion at end of isothermal section:',round(conv_space[end_idx_iso],3))
print('Volume of adibatic section:',round(vol_soln[end_idx_iso],3), 'm^3')
print('Total Volume:',round(vol_soln[end_idx_iso]+volume_space[end_idx_ad],3), 'm^3')
```

```
5714
Conversion at end of isothermal section: 0.8
Volume of adibatic section: 0.098 m^3
Total Volume: 0.244 m^3
```

Since

$$\Delta X_{isotherm} = 0.8 - 0.56 = 0.24$$

and the heat of reaction is -15000 J/mol, and $0.24 * 600 = 144 mol$ of A react, so

$$\Delta H = 2,160,000 \frac{J}{s}$$

Since the volume of the isothermal section is 0.098 m^3, the length is 49.91 m, making the surface area

$$SA = \pi * d * l = 7.84 m^2$$

$$Q = U \cdot A \cdot \Delta T$$

So assuming the coolant temperature is 25 $^\circ$C,

$$2160000 = U \cdot 7.84 m^2 \cdot 375 K$$

Solving for U,

$$U = 734 \frac{J}{m^2 \cdot s \cdot K}$$