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]) ]
```

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])
```

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)
```

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
```

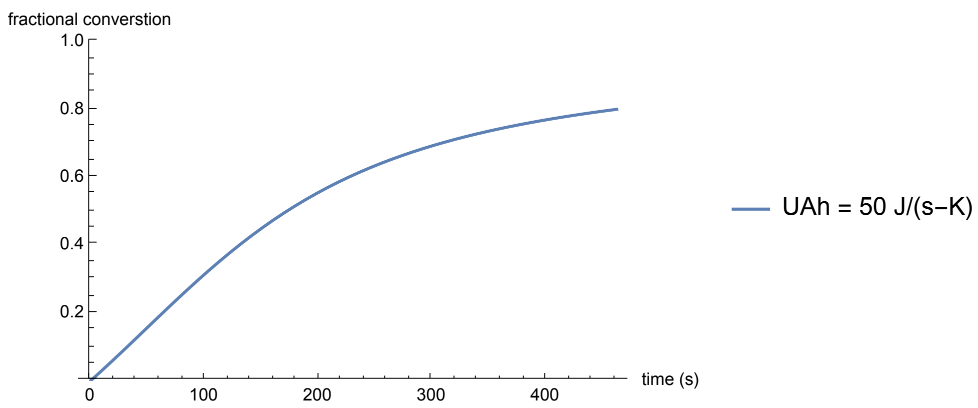
Out[∘]= 0.799805

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

Out[∘]= 331.623

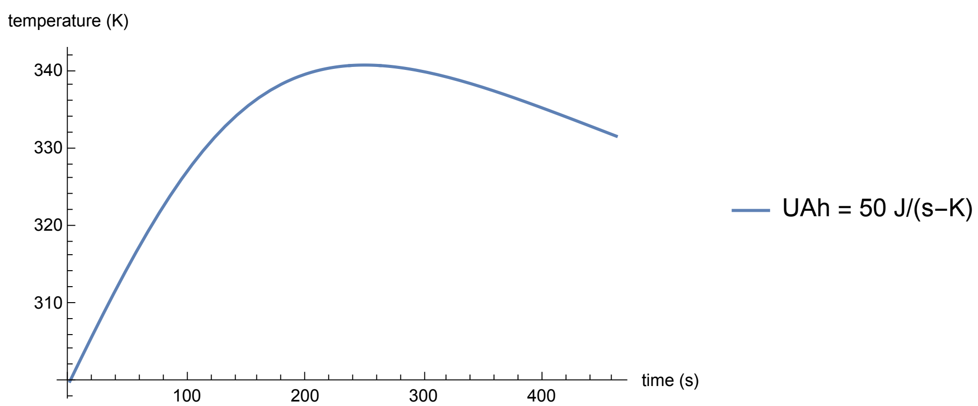
In[∘]:=
```
Plot[fa[t] /. answer[[1]], {t, 0, 462}, PlotRange → {0, 1},
 AxesLabel → {"time (s)", "fractional converstion"},
 PlotLegends → {"UAh = 50 J/(s-K)"}]
```

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[∘]= -741 582.

In[∘]:=
```
100 × .7925 × 15 000
```

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[∘]= 452 209.

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[∘]=

$$\frac{3750.\ e^{2405.58 \times \left(\frac{1}{300} - \frac{1}{T[t]}\right)} (1 - fa[t]) \times (1.2 - fa[t])}{6500 \times (1 - fa[t]) + 6500 \times (1.2 - fa[t]) + 15\,000\ fa[t]}$$

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
```

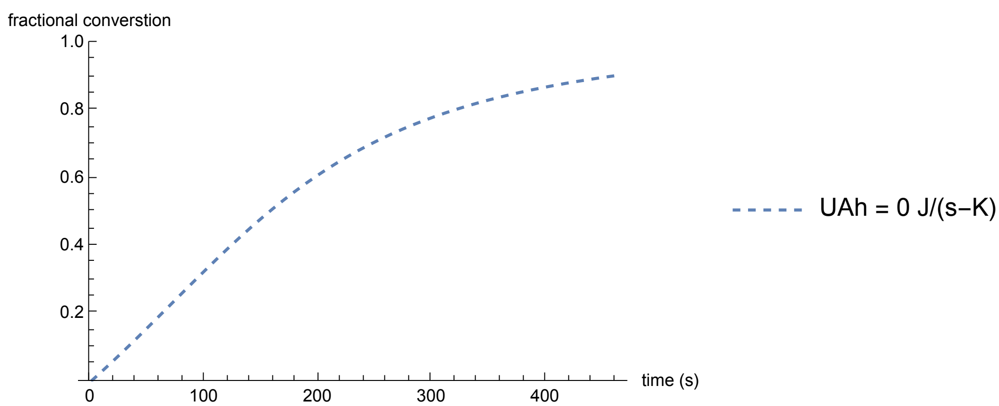
Out[∘]= 0.902252

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

Out[∘]= 389.13

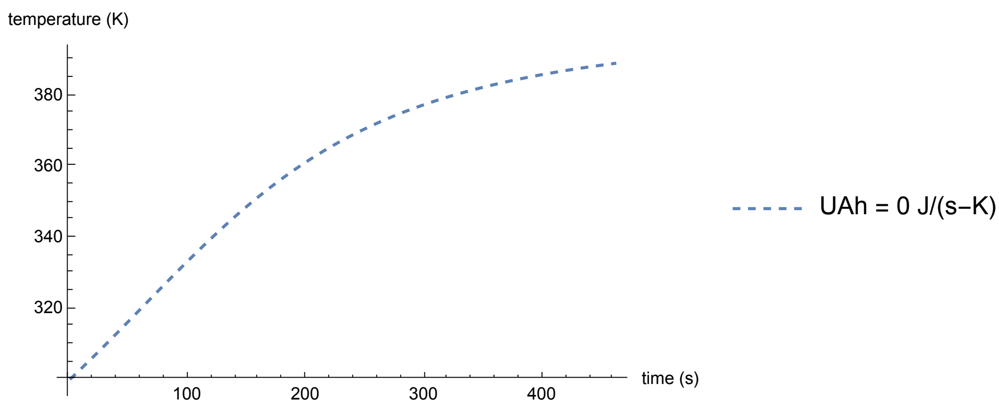
In[∘]:=
```
Plot[fa[t] /. hwanswer⟦1⟧, {t, 0, 462}, PlotRange → {0, 1},
 AxesLabel → {"time (s)", "fractional converstion"},
 PlotLegends → {"UAh = 0 J/(s-K)"}, PlotStyle → Dashed]
```

Out[∘]=



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

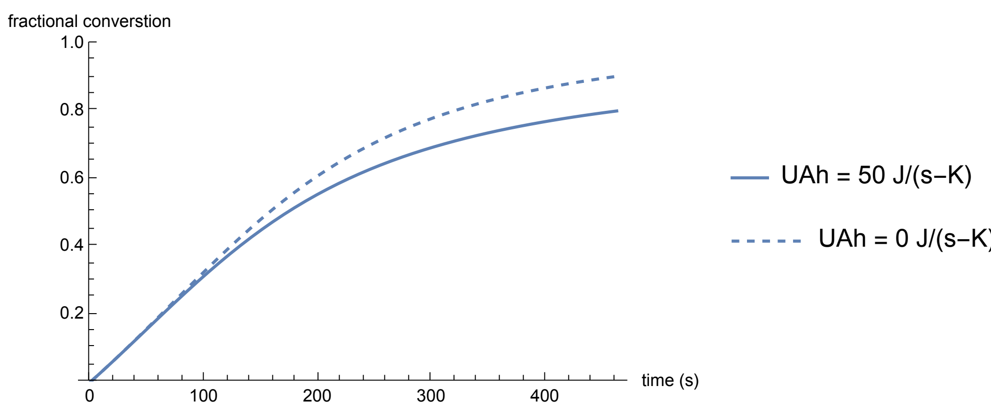
Out[•]=



Compare answers:

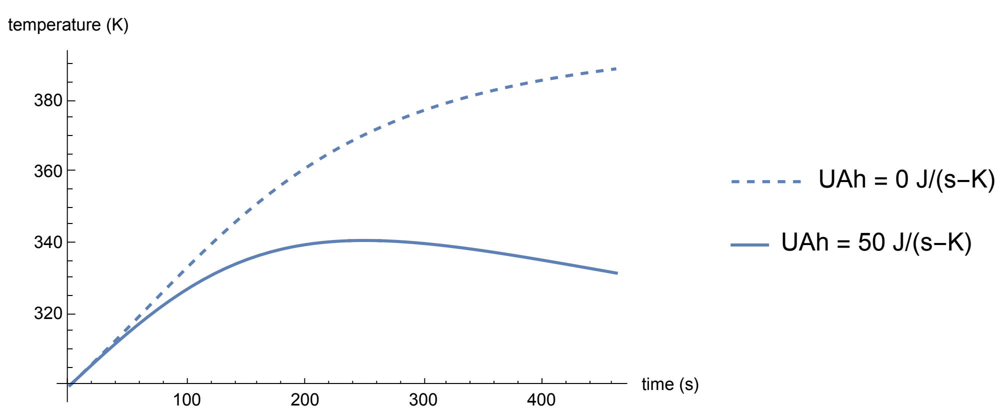
In[•]:=
```
Show[%351, %360]
```

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])]
```

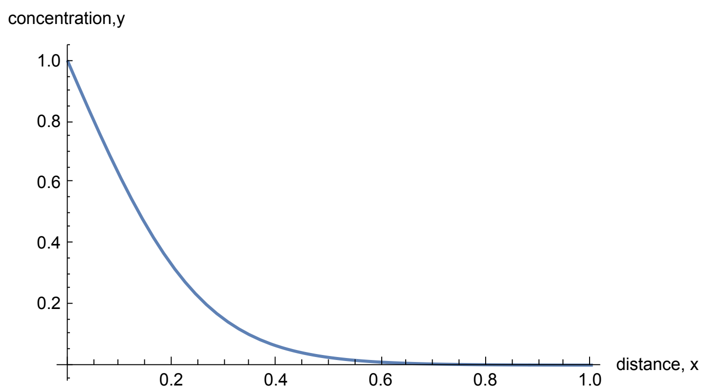
Out[∘]= $0.2\, e^{18 \times \left(1-\frac{1}{\theta[x]}\right)}\, y[x]$

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]}}
```

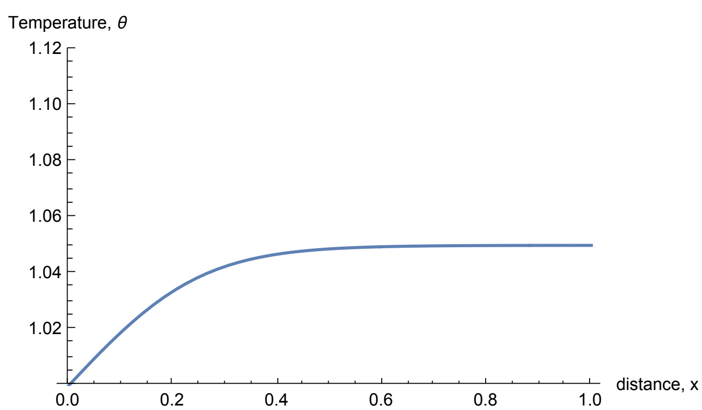
In[∘]:=
```
cans1 =
 Plot[y[x] /. ans3[[1]], {x, 0, 1}, AxesLabel → {"distance,  x", "concentration,y"}]
```

Out[∘]=



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

Out[∘]=



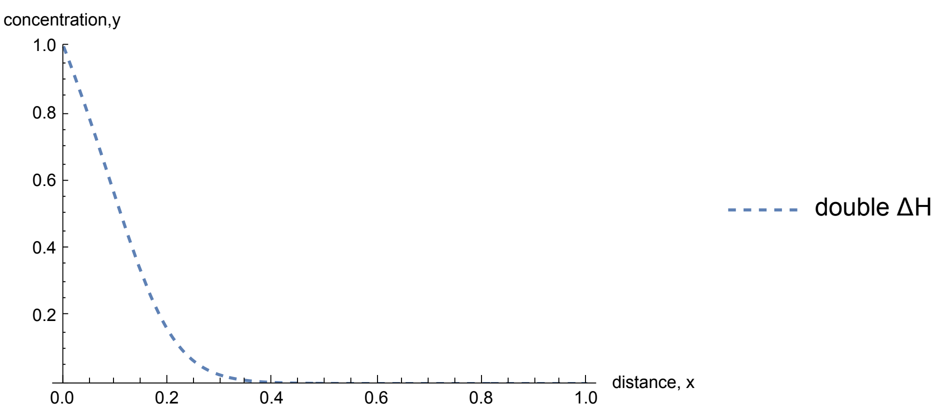
Redo with the heat reaction term doubled

In[∘]:=
```
massbalanceeq = - 4 y[x] Exp[ 18 ( 1 - 1 / θ[x])]
```
Out[∘]= $-4\, e^{18\times\left(1-\frac{1}{\theta[x]}\right)}\, y[x]$

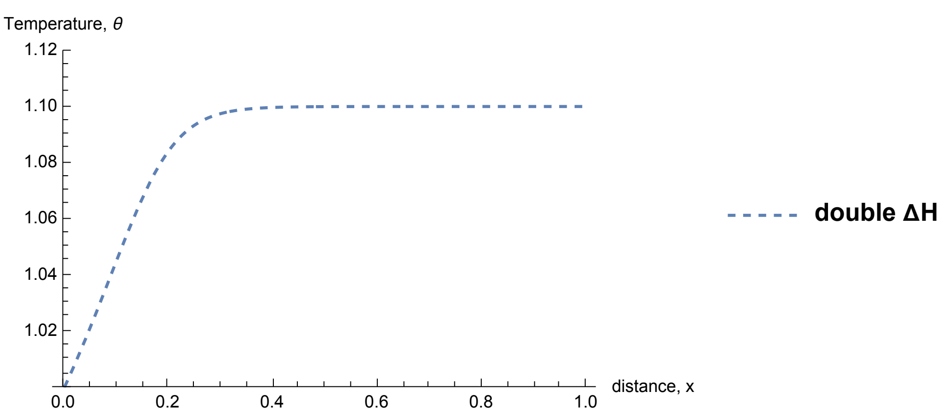
In[∘]:=
```
doubleenergybalanceeq =  .4 y[x] Exp[ 18 ( 1 - 1 / θ[x])]
```
Out[∘]= $0.4\, e^{18\times\left(1-\frac{1}{\theta[x]}\right)}\, y[x]$

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[∘]=

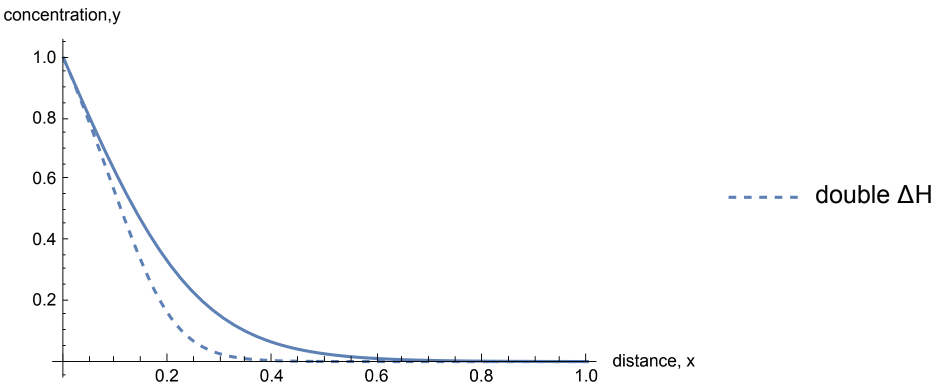


In[∘]:=
```
Plot[θ[x] /. ans3dbl[[1]], {x, 0, 1},
 AxesLabel → {"distance, x", "Temperature, θ"}, PlotRange → {1, 1.12},
 PlotStyle → Dashed, PlotLegends → {"double ΔH"}, PlotRange → {0, 1}]
```
In[∘]:=



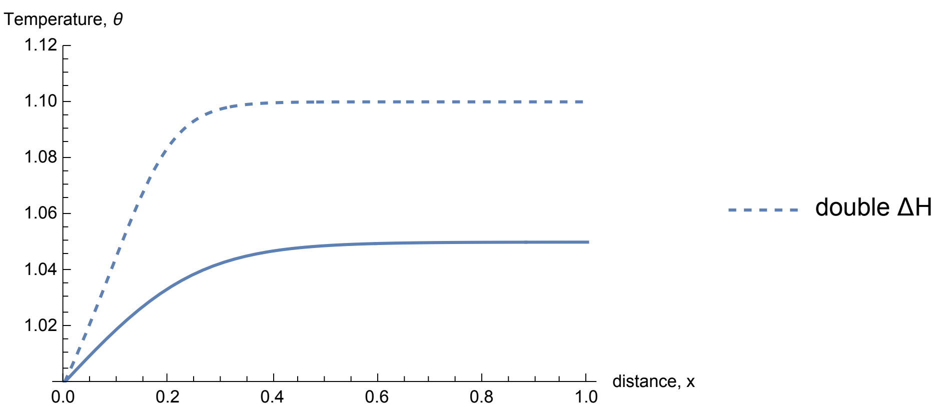
In[∘]:= `Show[%374, %381]`

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)
```

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

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]**

Out[∘]= $\left\{\left\{T \to \frac{30\ cp\ q - cef\ qef\ \triangle H}{cp\ q}\right\}\right\}$

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)]**

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

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

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

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

Out[∘]= $cp\ q\ (-303 + T) + cb\ ce\ k\ V\ \triangle H$

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

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

In[∘]:= **eqs = {eq11 , eq21, ebalance1 == 0}**

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

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

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

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.