Solutions to workshop 09: External diffusion effects

Lecture notes for chemical reaction engineering

Ranjeet Utikar

2024-03-24

P 14-9

The irreversible gas-phase reaction

$\text{A} \xrightarrow{\text{cat}} \text{B}$

is carried out adiabatically over a packed bed of solid catalyst particles. The reaction is first order in the concentration of A on the catalyst surface

$$-r'_{As} = k' C_{As}$$

The feed consists of 50% (mole) A and 50% inerts, and enters the bed at a temperature of 300 K. The entering volumetric flow rate is 10 dm^3/s (i.e., 10,000 cm^3/s). The relationship between the Sherwood number and the Reynolds number is

$$Sh = 100 Re^{1/2}$$

As a first approximation, one may neglect pressure drop. The entering concentration of A is 1.0 M. Calculate the catalyst weight necessary to achieve 60% conversion of A for

(a) isothermal operation.

(b) adiabatic operation.

Additional information:

- Kinematic viscosity: $\mu/\rho = 0.02 cm^2/s$
- Particle diameter: $d_p = 0.1 cm$
- Superficial velocity: $U = 10 cm/s$
- Catalyst surface area/mass of catalyst bed: $a = 60 cm^2/g - cat$
- Diffusivity of A: $D_e = 10^{-2} cm^2/s$
- Heat of reaction: $\Delta H^\circ_{Rx} = 10,000 cal/gmol A$
- Heat capacities: $C_{pA} = C_{pB} = 25 cal/gmol \cdot K, C_{pS}$ (solvent) $= 75 cal/gmol \cdot K$
- $k'(300K) = 0.01 cm^3/s \cdot g - cat$ with $E = 4000 cal/mol$

Solution

Hand written solution

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

# constants

RCAL = 1.987  # cal / mol K

# data
NU_VIS = 0.02 # cm^2/s
DP = 0.1  # cm
VEL = 10 # cm/s
SP_AREA = 60 # cm^2/g-cat
DE = 1e-2 # cm^2/s
DELTA_HR_TR = 10000 # cal/gmol A
CPA = 25 # cal/gmol K
CPB = 25 # cal/gmol K
CPS = 75 # cal/gmol K -- Solvent is inert

KA0 = 0.01 # cm^3/s g-cat
EA0 = 4000 # cal/mol
TR = 300 # K

# Functions
k = lambda t: KA0 * np.exp((EA0 / RCAL) * ((1 / TR) - (1 / t)))

def reactor(w, y, *args):
   # convert dependent variables
   x = y[0]
   (t0, ca0, fa0, phia, phis, kc) = args

   # isothermal case
   t = t0

   # Adiabatic case
   t = t0 + (x * DELTA_HR_TR / (phia * CPA + phis * CPS))

   ca = ca0 * (1-x) * (t0/t)
   rate =  k(t) * kc * ca / (k(t) + kc)

   dxdw = rate / fa0

   dydw = [dxdw]
   return dydw

# Problem data
ca0 = 1.0e-3 # mol/cm^3
v0 = 1.0e4 # cm^3/s
t0 = 300
phia = 1 # 50% A in inlet
phis = 1 # 50% A in inlet

Re = DP * VEL/ NU_VIS
Sh = 100 * Re**0.5
```

k_c = 4242.641 $cm^3/s\ g - cat$
C_{A0} = 0.001 mol/cm^3
F_{A0} = 10.000 mol/s
T_0 = 300.000 K
Catalyst weight required for X = 0.6: 538.539 kg
Temperature: 360.08 K

```
plt.plot(w/1000, x, label="conversion")
plt.xlim(w[0]/1000, w[-1]/1000)
plt.ylim(0, 1)
plt.grid()
plt.legend()

plt.xlabel("weight ($kg$)")
plt.ylabel("Conversion")

plt.show()
```

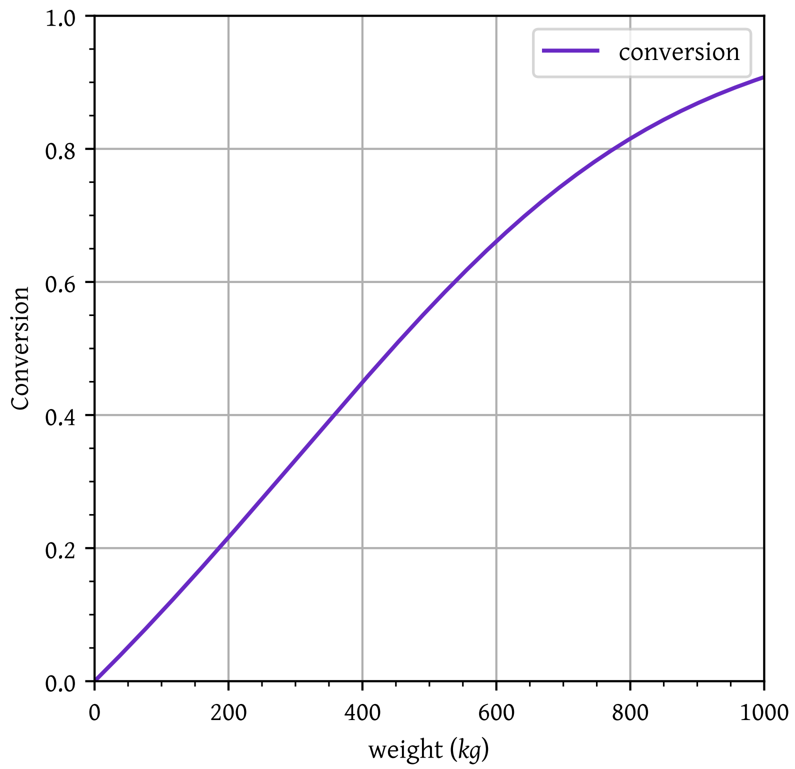

Figure 1: Conversion

```
plt.plot(w/1000, t, label="temperature")
plt.xlim(w[0]/1000, w[-1]/1000)
plt.ylim(t[0]-10, t[-1]+10)
plt.grid()
plt.legend()

plt.xlabel("weight ($kg$)")
plt.ylabel("Temperature ($K$)")

plt.show()
```

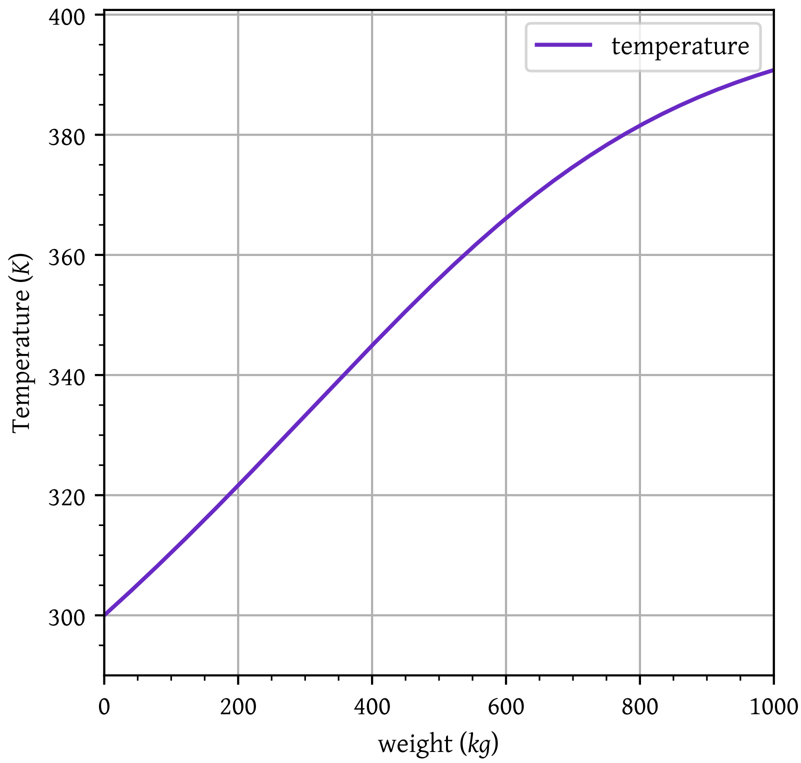

Figure 2: Temperature