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1
2 #+NAME: Yang Song
3 #+ANDREWID: yangsong
4 #+COURSE: 06-625
5 #+ASSIGNMENT: thiele-2
6 '''The reaction A  $\rightarrow$  B occurs in a packed bed reactor. Given
7 this additional information:
8
9  $r = k C_A^2$        $k = 2.25e5 \text{ cm}^3/\text{mol/s}$     (note this is a volumetric not mass
10      based rate constant)
11 A is fed to the reactor at 10 mol/s
12 An inert gas is fed to the reactor at 10 mol/s
13 The total pressure is 4 atm, at 550 K.
14 d
15 The catalyst is a spherical pellet with a radius of 0.45 cm. the bed
16 density is 0.60 gm/cm3, and the catalyst occupies 88% of the
17 volume. The effective diffusivity of A is 0.008 cm2/s.
18
19 The effective rate is given by:
20  $r_{eff} = \text{vol\_fraction} * \eta * r$ 
21
22 a) Estimate the mass of catalyst required to achieve 75% conversion of A
23 b) Plot the effectiveness factor as a function of catalyst weight
24 '''
25 import numpy as np
26 from pycse import BVP_nl
27 from scipy.integrate import odeint
28 k = 2.25e5 # cm3/mol/s
29
30 FA0 = 10.0 # mol/s
31
32 FI = 10.0 # mol/s
33
34 P = 4.0 # atm
35
36 T = 550.0 # K
37
38 R = 0.45 # cm
39
40 PA0 = P * FA0 / (FA0 + FI)
41 gas_const = 82.057 # atm*cm3/mol/K
42
43 CA0 = PA0 / gas_const / T # mol/cm3
44
45 v = (FI + FA0) * gas_const * T / P # cm3/s, is a constant throughout the
46      reactor.
47
48 phi = 1 - 0.88 # porosity
49
50 De = 0.008 # cm2/s
51
52 a = R / 3.0 # reduced radius of catalyst pellet.
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52
53 roub = 0.6 # g/cm^3
54
55
56 # Method 1: Using BVP solver in pycse to solve /eta as a function of CAS.
57
58 # Problem (a)
59
60 def eta_calc(CAS):
61     R = 3.0
62     r1 = 0.0
63     r2 = R
64     N = 100
65     RBAR = np.linspace(r1, r2, N)
66     thiele = np.sqrt(1.5 * k * CAS * a ** 2 / De)
67     p = 4
68     c0 = 0.9
69     init = c0 + (1 - c0) / R**p * RBAR**p
70     def F(rbar, cbar, dcbardrbar):
71         return -2.0 / rbar * dcbardrbar + 2.0 / (2.0 + 1.0) * thiele**2 * cbar
72         **2.0
73
74     def BCS(rbar, cbar):
75         return [(cbar[1]-cbar[0])/(rbar[1]-rbar[0]), cbar[-1]-1]
76
77     CBAR = BVP_n1(F, RBAR, BCS, init)
78     eta = 1./9. * np.trapz(CBAR**2 * RBAR**2, RBAR)
79     return eta
80
81 def dVdFA(V, FA):
82     CAS = FA / v
83     r = k * CAS ** 2.0
84     eta = eta_calc(CAS)
85     reff = (1-phi) * eta * r
86     dVdFA = - 1.0 / reff
87     return dVdFA
88
89 FAexit = (1 - 0.75) * FA0
90 FAspan = np.linspace(FA0, FAexit)
91 sol = odeint(dVdFA, 0, FAspan)
92 W = roub * sol[-1, 0]
93 print 'Mass of the catalyst required to achieve 75% conversion of A is {0} g.'
94     .format(W)

```

Mass of the catalyst required to achieve 75% conversion of A is
219646.687638 g.

```

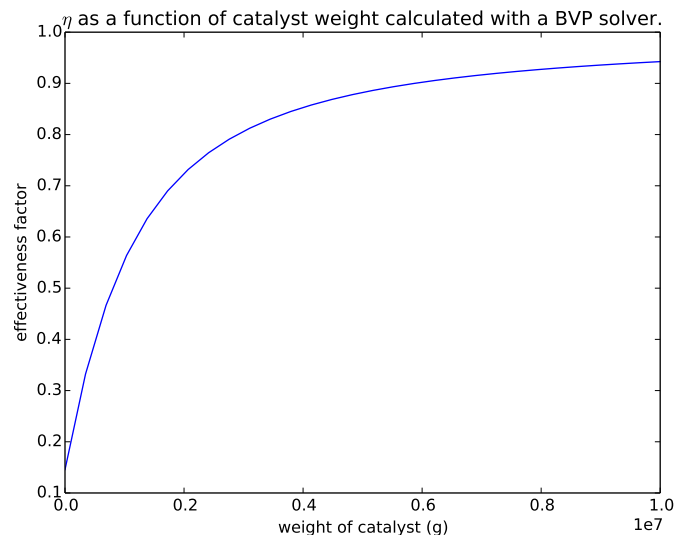
81
82 # Problem (b)
83
84 def dFAdV(FA, V):
85     CAS = FA / v
86     r = k * CAS ** 2.0
87     eta = eta_calc(CAS)
88     reff = (1-phi) * eta * r

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89     dFAdV = -reff
90     return dFAdV
91
92 Wspan = np.linspace(0, 1e7, 30)
93 ETA = np.empty(Wspan.shape)
94 Vspan = Wspan / roub
95 FA = odeint(dFAdV, FA0, Vspan)
96 CAS = FA / v
97 for i, CASi in enumerate(CAS):
98     ETA[i] = eta_calc(CASi)
99
100 import matplotlib.pyplot as plt
101 plt.figure()
102 plt.plot(Wspan, ETA)
103 plt.xlabel('weight of catalyst (g)')
104 plt.ylabel('effectiveness factor')
105 plt.title('η as a function of catalyst weight calculated with a BVP solver.')
106 plt.show()

```



```

107
108 # Method 2: using the analytical solution of η for 1st-order, spherical
109 # particles.
110 # The error should be tolerable.
111 # Problem (a)
112 def dVdFA(V, FA):
113     CAS = FA / v
114     r = k * CAS ** 2.0
115     thiele = np.sqrt(1.5 * k * CAS * a**2 / De)
116     eta = 1.0 / thiele * (1.0 / np.tanh(3*thiele) - 1.0 / (3.0*thiele))
117     reff = (1-phi) * eta * r
118     dVdFA = - 1.0 / reff
119     return dVdFA
120
121 FAexit = (1 - 0.75) * FA0
122 FAspan = np.linspace(FA0, FAexit)

```

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123 sol = odeint(dVdFA, 0, FAspan)
124 W = rouB * sol[-1, 0]
125 print 'Mass of the catalyst required to achieve 75% conversion of A is {0} g.'
    .format(W)

```

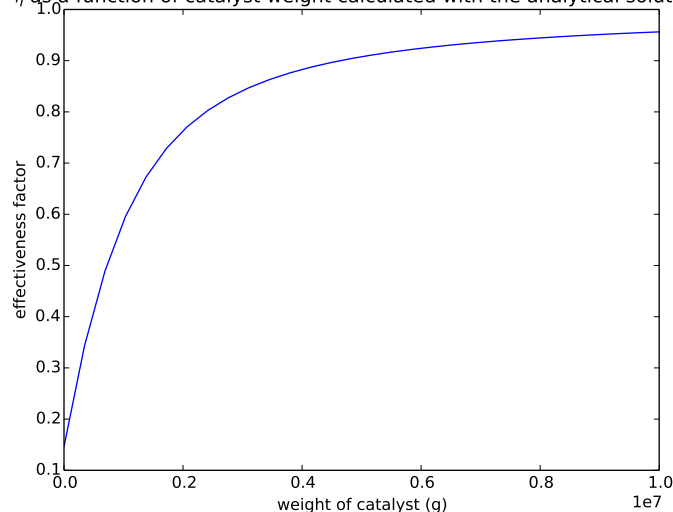
Mass of the catalyst required to achieve 75% conversion of A is
216933.061881 g.

```

126
127 # Problem (b)
128 def dFAdV(FA, V):
129     CAS = FA / v
130     r = k * CAS ** 2.0
131     thiele = np.sqrt(1.5 * k * CAS * a**2 / De)
132     eta = 1.0 / thiele * (1.0 / np.tanh(3*thiele) - 1.0 / (3.0*thiele))
133     reff = (1-phi) * eta * r
134     dFAdV = -reff
135     return dFAdV
136
137 Wspan = np.linspace(0, 1e7, 30)
138 ETA = np.empty(Wspan.shape)
139 Vspan = Wspan / rouB
140 FA = odeint(dFAdV, FA0, Vspan)
141 CAS = FA / v
142 for i, CASi in enumerate(CAS):
143     thiele = np.sqrt(1.5 * k * CASi * a**2 / De)
144     ETA[i] = 1.0 / thiele * (1.0 / np.tanh(3*thiele) - 1.0 / (3.0*thiele))
145
146 import matplotlib.pyplot as plt
147 plt.figure()
148 plt.plot(Wspan, ETA)
149 plt.xlabel('weight of catalyst (g)')
150 plt.ylabel('effectiveness factor')
151 plt.title('η as a function of catalyst weight calculated with the analytical
    solution.')
152 plt.show()

```

η as a function of catalyst weight calculated with the analytical solution.



153

154 *# We can see the two methods yield very close results, indicating the BVP
solver works well with this problem.*

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