```python

#+NAME: Yang Song
#+ANDREWID: yangsong
#+COURSE: 06-625
#+ASSIGNMENT: thiele-1
'''A first-order heterogeneous, irreversible reaction is taking place within a spherical catalyst pellet coated with catalyst. The reactant concentration halfway  between the outer surface and the center of the pellet (r = R/2) is equal to 1/10th of the surface concentration. The surface concentration is 0.001 mol / L, the particle diameter is 2e-3 cm, and the diffusion coefficient is 0.1 cm^2 / s.

a) Estimate the effectiveness factor of this catalyst particle
b) What diameter should the particle be decreased to get an effectiveness factor of 0.8. Provide an assessment of your answer.
'''

import numpy as np
from scipy.optimize import fsolve
CAs = 0.001 # mol / L

R = 1.e-3 # cm

De = 0.1 # cm^2 / s, diffusivity

a = R / 3.0 # characteristic length scale defined by the volume to surface ratio for a sphere.

# Define dimensionless radius as r_ = r / a, dimensionless concentration as c_ = CA / CAs
# The reaction is first-order and irreversible, assume it is elementary, then the analytical solution for catalytical reaction in a spherical catalyst particle is:
# c_ = (3 * sinh(phi) * r) / (r_ * sinh(3 * phi))
# The effectiveness factor is : eta = 1 / phi * (1 / tanh(3 * phi) - 1 / (3 * phi))
# Where phi is the Thiele modulus, defined as phi = sqrt(k * a^2 / De), k is the rate constant.

# Note: the above two analytical solutions are adapted from Dr. Kitchin's note part 4 page 17.

# We know at r_ = R/2 / a, c_ = CA / CAs = 0.1
def func(phi):
    eq1 = 0.1 - (3 * np.sinh(phi * R / 2 / a)) / (R / 2 / a * np.sinh(3 * phi))
    return eq1

guess = [0.5]
sol, = fsolve(func, guess)
phi = sol

eta = 1.0 / phi * (1.0 / np.tanh(3.0 * phi) - 1.0 / (3 * phi))
```

```
print 'Effectiveness factor of this catalyst particle is: {0}.'.format(eta)
```

```
Effectiveness factor of this catalyst particle is: 0.417427288901.
```

```

# We can know the rate constant now:
k = phi ** 2 * De / a ** 2

# We can find the radius of particle by using fsolve.
def func2(D):
    R = D / 2.0
    a = R / 3.0
    phi = np.sqrt(k * a ** 2 / De)
    eq1 = 0.8 - 1.0 / phi * (1.0 / np.tanh(3.0 * phi) - 1.0 / (3 * phi))
    return eq1

sol2, = fsolve(func2, [1.e-3])
print 'Diameter of the catalyst particle should be reduced to {0} cm.'.format(
    sol2)
```

```
Diameter of the catalyst particle should be reduced to 0.00068223386046 cm.
```

```

# When the particle diameter is reduced, mass transfer handicap is reduced and
    the concentration profile along the catalyst particle radius should be
   overall higher, making the catalyst working closer to ideal conditions
   that concentration at any position within the particle is equal to surface
    concentration. Therefore effectiveness factor is also higher.
```

```
hostname: yangsong-PC.home
ipaddr:   192.168.1.6
mac:      145169596412
```

Press to select grade Grade: