BP205 Molecular Dynamics of the Cell
Problem Set 3
Solutions

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1. Simulating a 1-dimensional reaction diffusion system.

a. $P_e = \frac{vd}{D}$

$d = 10^{-6} m; v = 30 * 10^{-6} \frac{m}{s}; D = 2 * 10^{-10} \frac{m^2}{s}$

$P_e = .15$

So, only diffusion is relevant.

Here is the code that I used for the rest of the problem:

```
function []  = bp205_prob_set_scratch()

init_conc = 1
init = init_conc*ones(50,1);
init(20:30) = 0;
stead_state = ones(91,1);

for diffus = 10:1:100

    [T conc] = ode45(@calc_conc2,[0,700],
init,odeset(),diffus);

    stead_state(diffus-9) = conc(end,1)

end


plot(stead_state)

end

function dconcdt = calc_conc2(t,y,diffus)

    dconcdt = ones(50,1);
   % diffus = 100;
    degrad = 1;
    grad = diffus*del2(y);
    dconcdt = y.^3./(.5^3+y.^3) - degrad*y + grad;

end
```

b. The steady state is 0 at all points

c. A steady state is .81 at all points

d. The steady state at all points is .81

e. The steady state at all points is 0

f. An abrupt crossover between the two regimes exist. The exact location of the cross-over seemed to vary depending on the particulars of how the system was coded. (I saw 40, but others reported around 20 and around 80)

2)
I used these constants; answers will vary depending on values used.

$$Re_{e.coli} = 3 * 10^{-5} \qquad \rho_{water} = 10^{3} kg$$

$$L_{human} = 10^{0} m \qquad \eta_{water} = 10^{-3} \frac{kg}{ms}$$

$$v_{human} = 10^{0} \frac{m}{s}$$

a. $$v = \frac{Re * \eta}{\rho * L} = 3 * 10^{-11} \frac{m}{s}$$

b. $$L = \frac{Re * \eta}{\rho * v} = 3 * 10^{-11} m$$

c. $$\rho = \frac{\eta * Re}{L * v} = 3 * 10^{-8} \frac{kg}{m^3}$$