10.34 Quiz 1, October 4, 2006

A perfectly-stirred reactor (a CSTR) is loaded with cells which multiply at a rate:

Cell Multiplication =
$$\frac{k_1 N_{cells} [Nutrients]}{(1 + c_1 [Nutrients])(1 + d[P])}$$

So the net balance on cells in the CSTR is:

$$\frac{dN_{cells}}{dt} = Cell Multiplication - Rate at which cells flow out of reactor$$

A nutrient/water mixture with [Nutrients]_{in} = 0.2 M is flowed into the 150 liter CSTR at a rate of 2.3 liter/min. The cells in the CSTR eat some of the nutrients:

Nutrient Consumption Rate = $k_2 N_{cells} + c_2$ (Cell Multiplication)

and produce a desired pharmaceutical product P:

$$P \text{ production rate} = \frac{k_3 N_{\text{cells}} \exp(-d[P])}{(1 + c_1 [\text{Nutrients}])} \cdot ([\text{Nutrients}] - 0.01)^2$$

The parameters are :

$$\begin{aligned} k_1 &= 0.5 & M^{-1} s^{-1} & c_1 &= 0.1 & M^{-1} \\ k_2 &= 1 \times 10^{-7} & moles \ cell^{-1} s^{-1} & c_2 &= 1 \times 10^{-5} \ moles \ cell^{-1} \\ k_3 &= 1 \times 10^{-6} \ moles \ cell^{-1} s^{-1} M^{-1} & d &= 0.01 & M^{-1} \end{aligned}$$

- (a) Write a couple of Matlab functions that together compute the concentrations [P] and [Nutrients] (units: M = moles/liter), as well as the number of cells per liter, in the output stream when the system is operated at steady-state. Give numerical values for all the inputs. Do you think that scaling will be a problem? Explain and give an appropriate scaling factor if necessary.
- (b) If your program from part (a) works correctly, how would you test whether the solution found is physical and achievable (i.e. stable)? (Explain in words; bonuses for giving correct relevant equations and/or Matlab functions).
- (c) If your program from part (a) converges to an unphysical or unstable solution, what would you do next to try to find an experimentally-relevant steady-state solution? (Explain in words; bonuses for giving correct relevant equations and/or Matlab functions.)

For your convenience, on the next page we have supplied the Matlab functions Cell_Multiplication.m, Nutrient_Consumption.m, P_production.m, and param_set.m, which you can call with the functions you write yourself. You can also call any built-in functions in Matlab and any functions presented as examples in class.

```
function CMrate = Cell Multiplication(Ncells,Nutrients,P,params)
% computes the Cell Multiplication rate (cells/s) in the CSTR
% inputs:
ò
   Ncells
                number of cells in the CSTR
   Nutrients
                concentration of Nutrients in the CSTR (moles/liter)
0
                concentration of Product in CSTR, [=] moles/liter
8
   Ρ
%
                values of [k1,k2,k3,c1,c2,d] as listed in problem statement.
  params
k1 = params(1); c1=params(4); d=params(6);
CMrate = k1.*Ncells.*Nutrients./((1+c1.*Nutrients).*(1+d.*P));
```

```
function NCrate = Nutrient Consumption(Ncells, Nutrients, P, params)
% computes the nutrient consumption rate in the CSTR (moles/s)
% inputs:
%
   Ncells
                 number of cells in the CSTR
                 concentration of Nutrients in the CSTR (moles/liter)
%
   Nutrients
ŝ
   Ρ
                 concentration of Product in CSTR, [=] moles/liter
8
   params
                 values of [k1,k2,k3,c1,c2,d] as listed in problem
statement.
k2 = params(2); c2 = params(5);
NCrate = k2*Ncells + c2*Cell Multiplication(Ncells,Nutrients,P,params);
```

```
function Prate = P_production(Ncells,Nutrients,P,params)
% computes the product production rate in the CSTR (moles/s)
% inputs:
   Ncells
                 number of cells in the CSTR
8
  Nutrients
                 concentration of Nutrients in the CSTR (moles/liter)
8
                 concentration of Product in CSTR, [=] moles/liter
%
   Ρ
                 values of [k1,k2,k3,c1,c2,d] as listed in problem
%
   params
statement.
k3 = params(3); d=params(6); c1=params(4);
Prate = k3.*Ncells.*exp(-d.*P).*((Nutrients-0.01).^2)./(1+c1.*Nutrients)
```

```
function params = param_set
% sets params as in the problem statement
% [k1 k2 k3 c1 c2 d]
params = [0.5 1e-7 1e-6 0.1 1e-5 0.01];
```