Grayson Gerlich **10801535** **Homework #2 Lab**

Systems Biology, Computer Lab # 1: Chemical Reaction Models

1. Reaction rates:

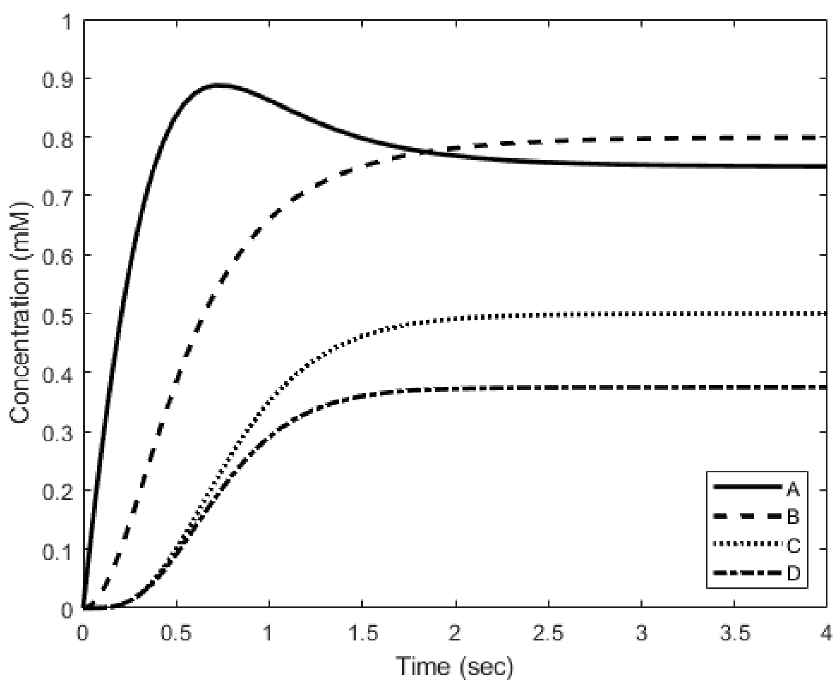
$$v_1 = k_1$$

$$v_2 = k_2 * [A]$$
$$v_3 = k_3 * ([A] * [B])$$
$$v_4 = k_4 * [C]$$
$$v_5 = k_5 * [D]$$

2. Differential Equations:

$$\frac{da}{dt} = k_1 - k_2 * a - k_3 * (a * b)$$
$$\frac{db}{dt} = k_2 * a - k_3 * (a * b)$$
$$\frac{dc}{dt} = k_3 * (a * b) - k_4 * c$$
$$\frac{dd}{dt} = k_3 * (a * b) - k_5 * d$$

3. Plot of solutions



4. Description of Dynamics: A is generated immediately, and A production drives production of B. Because the production of C and D is linked to both A and B, the populations of C and D increase on a sigmoid curve only once A and B concentrations are sufficient to drive the equilibrium. All species approach steady state and hold, except for A, which overproduces until C/D production begins and drives it to its steady state.

5. Determine the steady-state concentrations using your numerical solutions.

$$A = 0.7503$$

$$B = 0.7991$$

$$C = 0.5$$

$$D = 0.3750$$

6. Function Code

```
function dYdt = lab1_model(t,Y)  % TODO - Write the function declaration.
    % Name of the function is lab1_model
    % TODO - Extract a, b, c, and d from input vector Y
    a = Y(1); % a
    b = Y(2); % b
    c = Y(3); % c
    d = Y(4); % d

    % TODO - Define the constants k1 through k5
    k1 = 3; %mM/s
    k2 = 2; %1/s
    k3 = 2.5; %1/(mM*s)
    k4 = 3; %1/s
    k5 = 4; %1/s

    % TODO - Define dadt, dbdt, dcdt, dddt from the ODEs
    dadt = k1 - (k2*a) - (k3*(a*b));
    dbdt = (k2*a) - (k3*(a*b));
    dcdt = (k3*(a*b)) - (k4*c);
    dddt = (k3*(a*b)) - (k5*d);

    % Create output column vector dYdt
    dYdt = [dadt; dbdt; dcdt; dddt];
end
```

7. Driver Code

```
clear all

% TODO define the timespan to simulation
tRange = [0 4];

% TODO define the initial conditions
Y0 = zeros(1,4);

% call the solver of choice (ode45 is fine)
[tSol,YSol] = ode15s(@lab1_model,tRange,Y0);

```

```
% plot solutions to look like figure in lab

plot(tSol,YSol(:,1),'-k','LineWidth',2)
hold on
plot(tSol,YSol(:,2),'--k','LineWidth',2)
plot(tSol,YSol(:,3),':k','LineWidth',2)
plot(tSol,YSol(:,4),'-.k','LineWidth',2)
legend('A','B','C','D','Location','southeast')
xlabel('Time (sec)')
ylim([0 1]);
ylabel('Concentration (mM)')
```