BEBI5009 Homework1
Due 03/27/2018(Tue) before noon

1. **2.4.7 Network Modelling.**
Consider the closed reaction network in Figure 2.16 with reaction rates v_i as indicated. Suppose that the reaction rates are given by mass action as $v_1 = k_1[A][B]$, $v_2 = k_2[D]$ and $v_3 = k_3[C]$.
(1) Construct a differential equation model for the network. Use moiety conservations to reduce your model to three differential equations and three algebraic equations.
(2) Solve for the steady-state concentrations as functions of the rate constants and the initial concentrations. (Note, because the system is closed, some of the steady-state concentrations are zero.)
(3) Verify your result in part (2) by running a simulation of the system from initial conditions (in mM) of ([A], [B], [C], [D], [E], [F]) = (1, 1, 0.5, 0, 0, 0).
Take rate constants k_1 = 3/mM/sec, k_2 = 1/sec, k_3 = 4/sec.

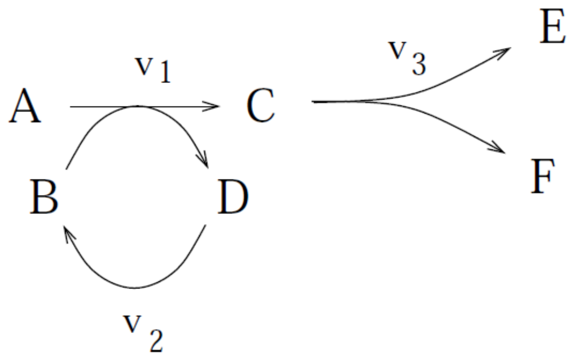

Figure 2.16: Closed reaction network for Problem 2.4.7(a).

2. Numerical method: **Fourth-Order Runge-Kutta Method (RK4)**
Ref: Chapter 7, Numerical Methods in Engineering with Python 3 by Jaan Kiusalaas (2011)

Euler's method is based on the truncated Taylor series of **y** about *x*:

$$\mathbf{y}(x+h) \approx \mathbf{y}(x) + \mathbf{y}'(x)h \qquad \text{Eq.(1)}$$

Because Eq.(1) predicts **y** at *x* + *h* from the information available at *x*, it can be used to move the solution forward in steps of *h*, starting with the given initial values of *x* and **y**. The error in Eq. (1) caused by truncation of the Taylor series is given by

$$\mathrm{E} = \frac{1}{2}\mathrm{y}''(\xi)h^2,$$

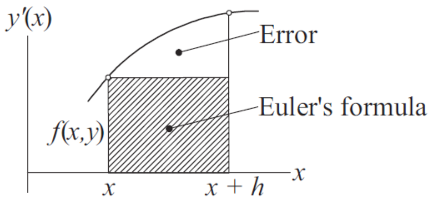

Figure 7.1. Graphical representation of Euler's formula.

Euler's method is seldom used in practice because of its computational inefficiency. Suppressing the truncation error to an acceptable level requires a very small h, resulting in many integration steps accompanied by an increase in the roundoff error. The value of the method lies mainly in its simplicity, which facilitates the discussion of certain important topics, such as stability.

The accuracy of numerical integration can be greatly improved by keeping more terms of the Taylor's series. *Runge-Kutta methods* that are based on truncated Taylor series, but do not require computation of higher derivatives of $\mathbf{y}(x)$. The most popular version is the forth order Runge-Kutta Method which entails the following sequence of operations:

$$K_0 = hF(x, y)$$

$$K_1 = hF\left(x + \frac{h}{2}, y + \frac{K_0}{2}\right)$$

$$K_2 = hF\left(x + \frac{h}{2}, y + \frac{K_1}{2}\right)$$

$$K_3 = hF(x + h, y + K_2)$$

$$y(x + h) = y(x) + \frac{1}{6}(K_0 + 2K_1 + 2K_2 + K_3) \qquad (Eq.2)$$

(1) Use the fourth-order Runge-Kutta method (Eq.2) to integrate the initial value problem as in Figure 2.7 the textbook:

$$\frac{d}{dy}a(t) = -a(t)$$

from $x = 0$ to 4 in increments of $h = 1/3$ and 2/3. The initial condition is a(0)=1. Plot the computed y together with the analytical solution.

(2) Compare the y computed y by Runge-Kutta method with the y computed by Euler method (Fig2-07 Euler method Matlab or Python codes could be downloaded in Gibhub:
https://github.com/SosirisTseng/BEBI-5009/tree/master/ch2).
You could also try different h values.