CENTRO UNIVERSITÁRIO DA FEI
MESTRADO EM ENGENHARIA QUÍMICA

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Resolução Lista de Exercícios 04
Métodos Matemáticos em Engenharia Química
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1) exemplo 5.5, p.331

Example 5.5: Solution of the Optimal Temperature Profile for Penicillin Fermentation. Apply the orthogonal collocation method to solve the two-point boundary-value problem arising from the application of the *maximum principle of Pontryagin* to a batch penicillin fermentation. Obtain the solution of this problem, and show the profiles of the state variables, the adjoint variables, and the optimal temperature. The equations that describe the state of the system in a batch penicillin fermentation, developed by Constantinides et al.[6], are:

Cell mass production: $$\frac{dy_1}{dt} = b_1 y_1 - \frac{b_1}{b_2} y_1^2 \qquad y_1(0) = 0.03 \tag{1}$$

Penicillin synthesis: $$\frac{dy_2}{dt} = b_3 y_1 \qquad y_2(0) = 0.0 \tag{2}$$

where y_1 = dimensionless concentration of cell mass
y_2 = dimensionless concentration of penicillin
t = dimensionless time, $0 \le t \le 1$.

The parameters b_i are functions of temperature, θ:

$$b_1 = w_1 \left[\frac{1.0 - w_2(\theta - w_3)^2}{1.0 - w_2(25 - w_3)^2} \right] \qquad b_2 = w_4 \left[\frac{1.0 - w_2(\theta - w_3)^2}{1.0 - w_2(25 - w_3)^2} \right]$$

$$b_3 = w_5 \left[\frac{1.0 - w_2(\theta - w_6)^2}{1.0 - w_2(25 - w_6)^2} \right] \qquad b_i \ge 0 \tag{3}$$

where $w_1 = 13.1$ (value of b_1 at 25°C obtained from fitting the model to experimental data)
$w_2 = 0.005$
$w_3 = 30°C$
$w_4 = 0.94$ (value of b_2 at 25°C)
$w_5 = 1.71$ (value of b_3 at 25°C)
$w_6 = 20°C$
θ = temperature, °C.

These parameter-temperature functions are inverted parabolas that reach their peak at 30°C for b_1 and b_2, at 20°C for b_3. The values of the parameters decrease by a factor of 2 over a 10°C change in temperature on either side of the peak. The inequality, $b_i \geq 0$, restricts the values of the parameters to the positive regime. These functions have shapes typical of those encountered in microbial or enzyme-catalyzed reactions.

The maximum principle has been applied to the above model to determine the optimal temperature profile (see Ref. [7]), which maximizes the concentration of penicillin at the final time of the fermentation, $t_f = 1$. The maximum principle algorithm when applied to the state equations, (1) and (2), yields the following additional equations:

The *adjoint equations*:

$$\frac{dy_3}{dt} = -b_1 y_3 + 2\frac{b_1}{b_2} y_1 y_3 - b_3 y_4 \qquad y_3(1) = 0 \tag{4}$$

$$\frac{dy_4}{dt} = 0 \qquad y_4(1) = 1.0 \tag{5}$$

The *Hamiltonian*:

$$H = y_3\left(b_1 y_1 - \frac{b_1}{b_2} y_1^2\right) + y_4(b_3 y_1)$$

The *necessary condition* for maximum:

$$\frac{\partial H}{\partial \theta} = 0 \tag{6}$$

Eqs. (1)-(6) form a two-point boundary-value problem. Apply the orthogonal collocation method to obtain the solution of this problem, and show the profiles of the state variables, the adjoint variables, and the optimal temperature.

Iremos criar duas funções, onde a primeira irá conter os valores de y1 e y2 em função de b1, b2 e b3. Como b1, b2 e b3 são funções da Temperatura T, a segunda função, ira calcular y1 e y2, em função da Temperatura. Logo após, será calculado y2, para diversas temperaturas através de um script.

Criação da Function para calculo de Y1 e Y2 em função da temperatura, tendo como argumento de entrada Y1, Y2, o tempo e Temperatura e como saída, Y1, Y2. Y1 e Y2 irá sair em função de T.

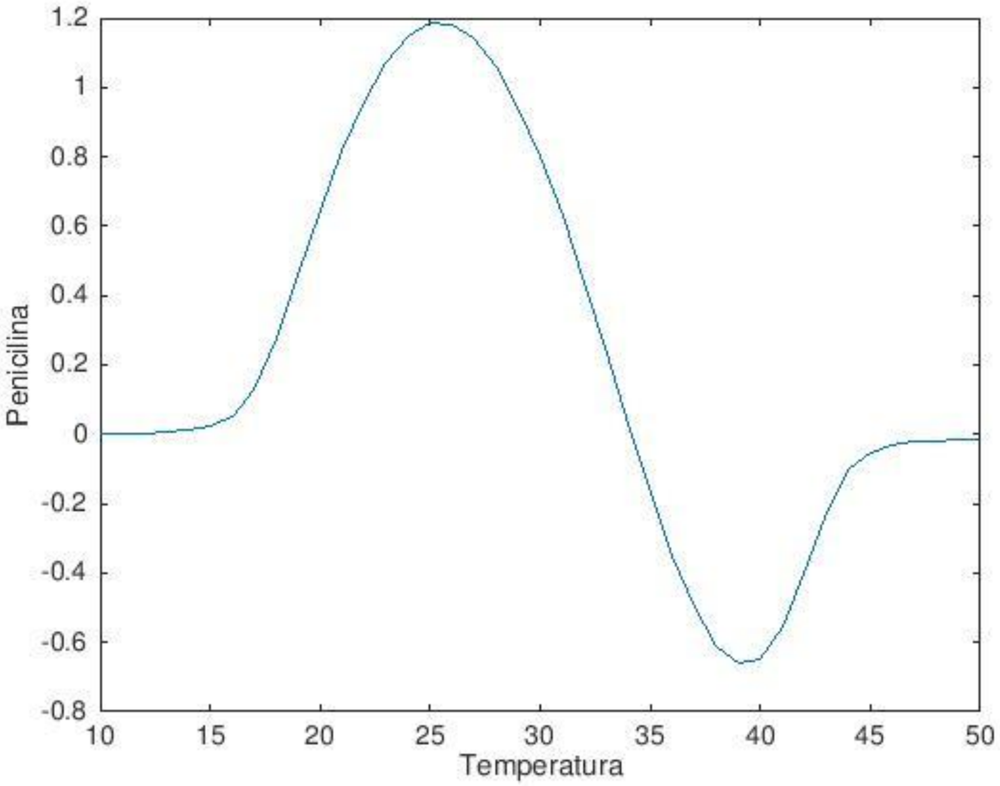
```
function f = Exercicio_1_fermentacao(t,x,T)
        w1=13.1;
        w2=0.005;
        w3=30;
        w4=0.94;
        w5=1.71;
        w6=20;
        T=x(3,1);
        b1=w1*((1-w2*(T-w3)^2)/(1-w2*(25-w3)^2));
        b2=w4*((1-w2*(T-w3)^2)/(1-w2*(25-w3)^2));
        b3=w5*((1-w2*(T-w6)^2)/(1-w2*(25-w6)^2));
        f=zeros(3,1);
        f(1)=b1*x(1,1)-(b1/b2)*x(1,1)^2;
        f(2)=b3*x(1,1);
        f(3)=0;
end
```

Criação da Function para calculo de Y1 e Y2, tendo como argumento de entrada a temperatura desejada T e como saída, o valor de Y2.

```
function f = Exercicio_1_Temperatura(T)
    x0 = [0.03;0;T];
    [t,x] = ode45('Exercicio_1_fermentacao',[0,1],x0);
    f = x(length(x),2);
end
```

Criação do Script para plotagem de Y2 em função da Temperatura. Como iremos ter vários valores de temperatura, iremos criar um For, que jogara na função Exercicio_1_Temperatura, varias temperaturas, e retornara como saída,vários valores de Y2 para varias temperaturas. Iremos armazenar o resultado de Y2 em uma variável, e plotar Y2 por T.

```
T =10:50';
x=zeros(length(T),1);
for i=1:length(T)
    x(i)=Exercicio_1_Temperatura(T(i));
end
plot(T,x)
ylabel('Penicilina')
xlabel('Temperatura')
```



Logo, a temperatura ótima se situa em 25ºC

2) exercício 5.3, p.354

5.3 A radioactive material (A) decomposes according to the series reaction:

$$A \xrightarrow{k_1} B \xrightarrow{k_2} C$$

where k_1 and k_2 are the rate constants and B and C are the intermediate and final products, respectively. The rate equations are

$$\frac{dC_A}{dt} = -k_1 C_A$$

$$\frac{dC_B}{dt} = k_1 C_A - k_2 C_B$$

$$\frac{dC_C}{dt} = k_2 C_B$$

where C_A, C_B, and C_C are the concentrations of materials A, B, and C, respectively. The values of the rate constants are

$$k_1 = 3\ \mathrm{s}^{-1} \qquad k_2 = 1\ \mathrm{s}^{-1}$$

Initial conditions are

$$C_A(0) = 1\ \mathrm{mol/m^3} \qquad C_B(0) = 0 \qquad C_C(0) = 0$$

(a) Use the eigenvalue-eigenvector method to determine the concentrations C_A, C_B, and C_C as a function of time t.

(b) At time $t = 1$ s and $t = 10$ s, what are the concentrations of A, B, and C?

(c) Sketch the concentration profiles for A, B, and C.

Realizando um Script em Matlab e utilizando o método analítico dado por:

$$x = M * e^{\lambda . t} * M^{-1} * x_0$$

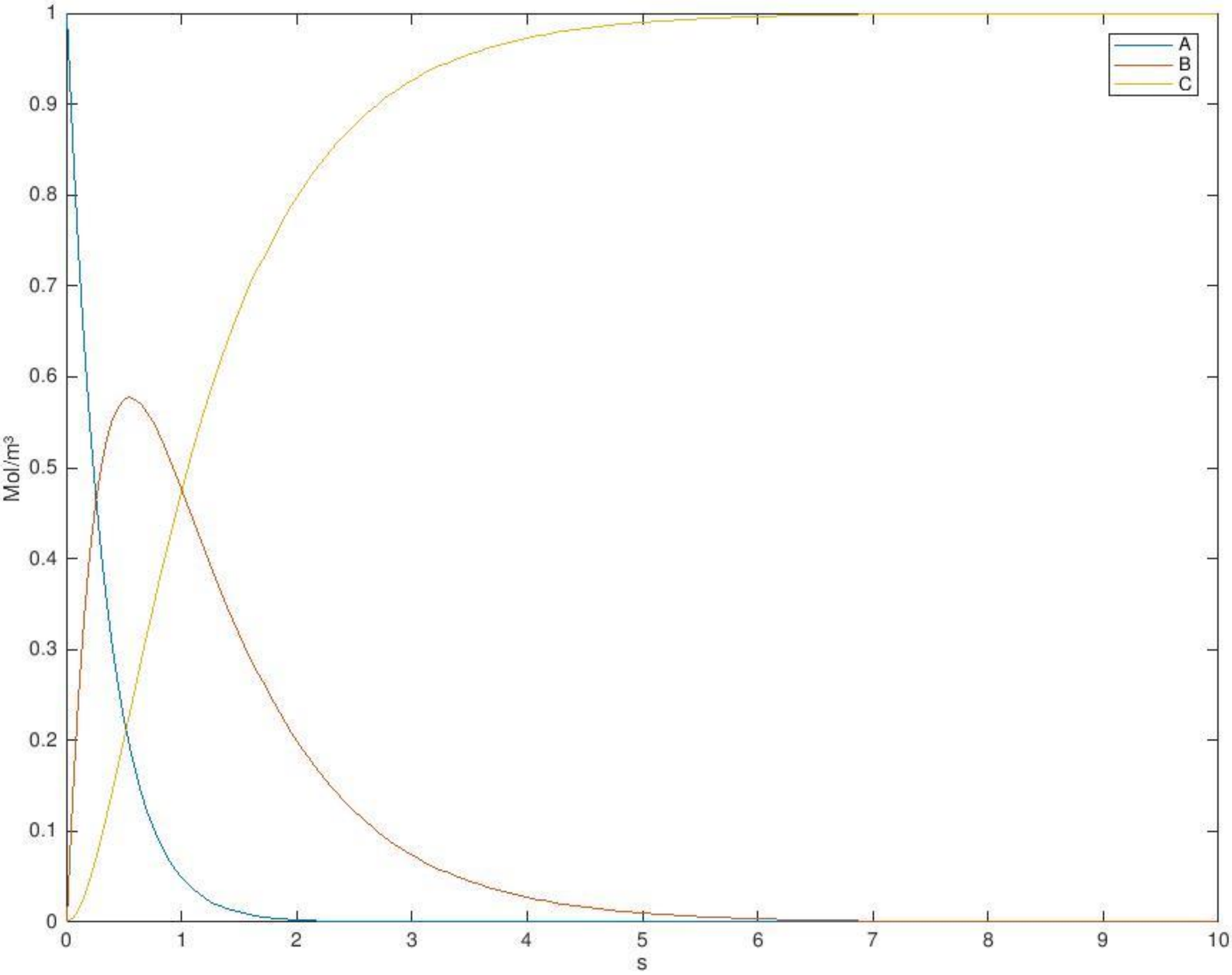
Onde, em Matlab, é calculado pela função EXPM(A*t), onde A é a matriz, e t é o escalar tempo.

Para descobrirmos as concentrações de A, B e C nos instantes 1 s e 10 s, realizaremos o uso da seguinte função:

```
x = expm(A*1)*x0


x =

    0.0498
    0.4771
    0.4731


x = expm(A*10)*x0


x =

    0.0000
    0.0001
    0.9999
```

Realizando um Script, para plotar as concentrações de A, B e C em função do tempo:

```
clear all
clc
k1=3;
k2=1;
A = [-k1,0,0;k1,-k2,0;0,k2,0];
h = 0.05;
x0 = [1;0;0];
t = 10;
i = 1;
for j = 0:h:t
    x(:,i) = expm(A*j)*x0;
    tempo(i) = j;
i = i+1;
end
x;
A=x(1,:)'
B =x(2,:)'
C =x(3,:)'
tempo'
plot(tempo,A)
hold on
plot(tempo,B)
plot(tempo,C)
xlabel('s')
ylabel('Mol/m³')
legend('A','B','C')
```



A
B
C
Mol/m³
s
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
1
2
3
4
5
6
7
8
9
10

3) exercício 5.4, p.355

5.4 (a) Integrate the following differential equations:

$$\frac{dC_A}{dt} = -4C_A + C_B \qquad C_A(0) = 100.0$$

$$\frac{dC_B}{dt} = 4C_A - 4C_B \qquad C_B(0) = 0.0$$

for the time period $0 \le t \le 5$, using (1) the Euler predictor-corrector method, (2) the fourth-order Runge-Kutta method.

(b) Which method would give a solution closer to the analytical solution?

(c) Why do these methods give different results?

Iremos escrever uma function em Matlab, dos balanços Molares de A e B

```
function f = Exercicio_3_btr(t,x)
    f = zeros(2,1);
    f(1,1) = -4*x(1,1) + 1*x(2,1);
    f(2,1) = 4*x(1,1) -4*x(2,1);
end
```

Em Seguida, iremos escrever uma function em Matlab, para o Método Número de Euler

```
function [t,y] = euler_expl(func,tspan,y0,h)
n = length(y0);
to = tspan(1);
tf = tspan(2);
t = (to:h:tf)';
y = zeros(n,length(t));
y(:,1) = y0;
for j = 2:length(t)
y(:,j) = y(:,j-1)+h*(feval(func,t(j-1),y(:,j-1)));
end
y = y';
```

Em Seguida, iremos escrever uma function em Matlab, para o Método de Runge-Kuta

```
function [t,y]  = rk4(func,tspan,y0,h)
n = length(y0);
to = tspan(1);
tf = tspan(2);
t = (to:h:tf)';
y = zeros(n,length(t));
y(:,1) = y0;
for j = 2:length(t)
dy1 = h*(feval(func,t(j-1),y(:,j-1)));
    dy2 = h*(feval(func,t(j-1),y(:,j-1)+(1/2)*dy1));
    dy3 = h*(feval(func,t(j-1),y(:,j-1)+(1/2)*dy2));
    dy4 = h*(feval(func,t(j-1),y(:,j-1)+dy3));
y(:,j) = y(:,j-1)+(1/6)*dy1+(1/3)*dy2+(1/3)*dy3+(1/6)*dy4;
end
y = y';
```

Com as funções escritas, iremos realizar os Scripts para os dois métodos.

Para o Método de Euler:

```
clear all
clc
h = 0.05;
tspan = [0,5];
y0 = [100;0];
[t,y] = euler_expl('Exercicio_3_btr',tspan,y0,h);
A = y(:,1)
B = y(:,2)
tempo = t
plot(tempo,A)
hold on
plot(tempo,B)
xlabel('h')
ylabel('Mol/m³')
legend('A','B')
```

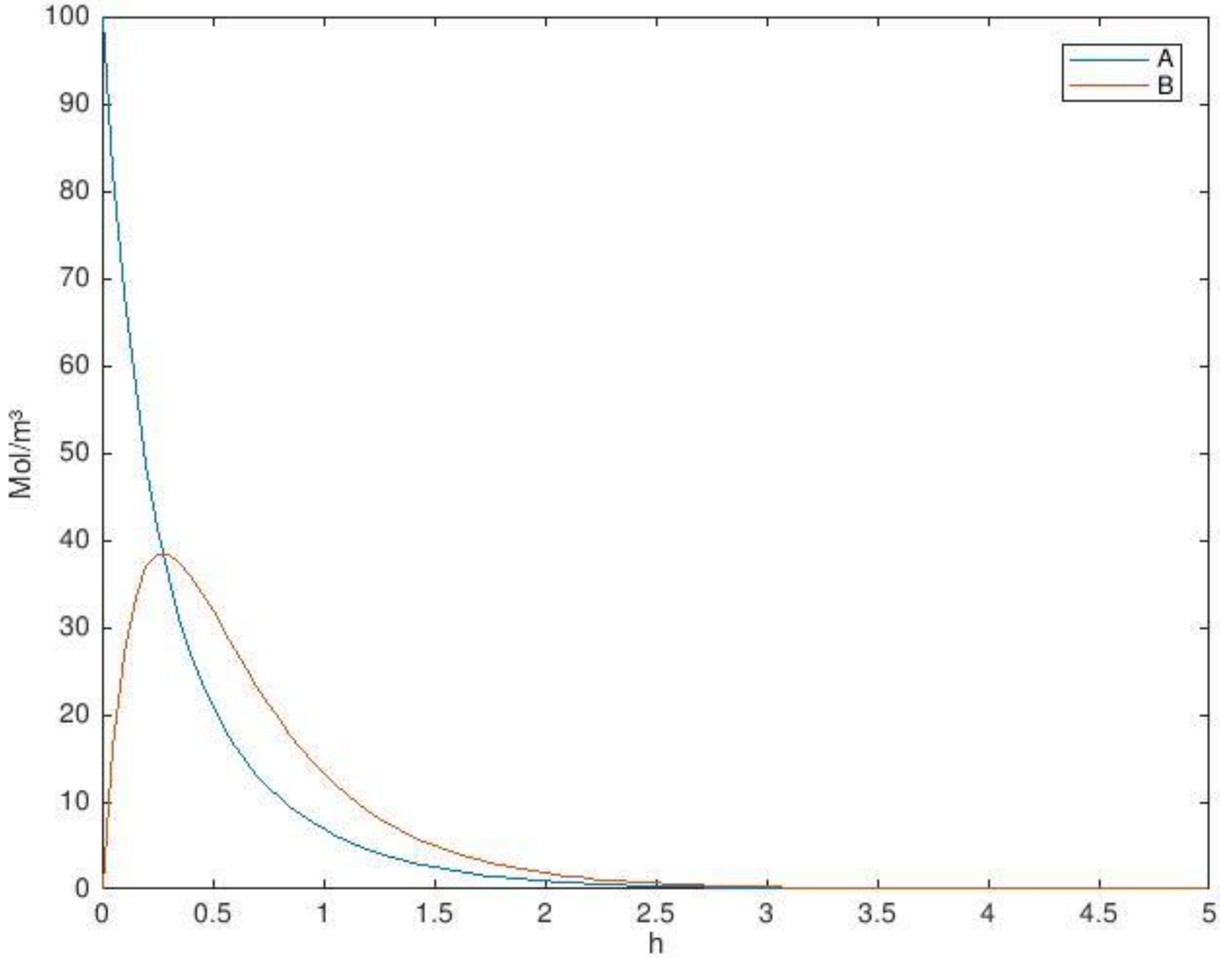
Para o Método de Runge-Kutta

```
clear all
clc
h = 0.05;
tspan = [0,5];
y0 = [100;0];
[t,y] = rk4('Exercicio_3_btr',tspan,y0,h);
A = y(:,1)
B = y(:,2)
tempo = t
plot(tempo,A)
hold on
plot(tempo,B)
xlabel('h')
ylabel('Mol/m³')
legend('A','B')
```

Para o Método Analitico:

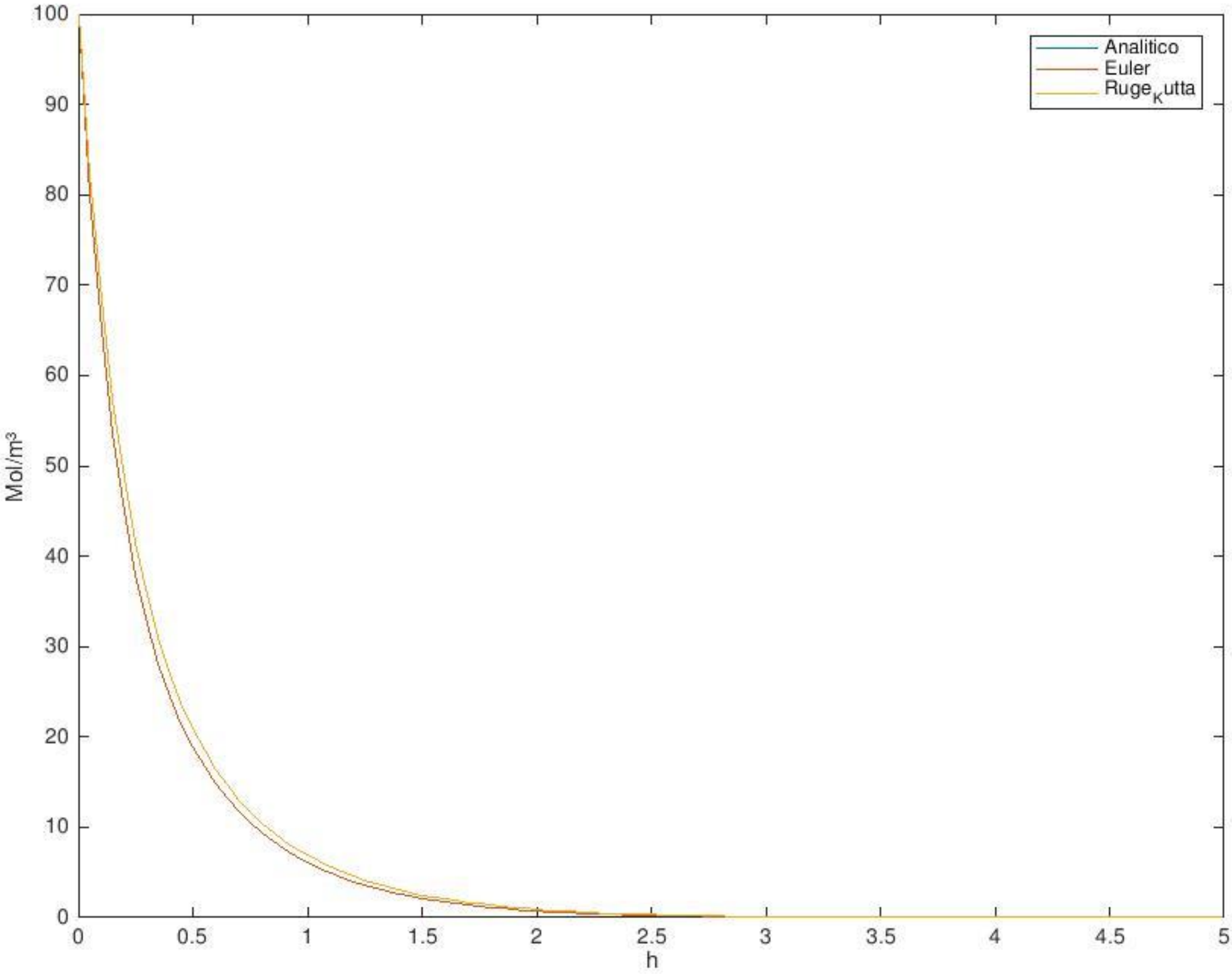
```
clear all
clc
A = [-4,1;4,-4];
h = 0.05;
x0 = [100;0];
t = 5;
i = 1;
for j = 0:h:t
    x(:,i) = expm(A*j)*x0;
    tempo(i) = j;
i = i+1;
end
x;
A=x(1,:)'
B =x(2,:)'
tempo'
plot(tempo,A)
hold on
plot(tempo,B)
xlabel('h')
ylabel('Mol/m³')
legend('A','B')
```

Abaixo, o Gráfico do Método Analítico:



Iremos comparar os valores da concentração de A, no gráfico, em relação ao Método de Euler, Método de Runge-Kutta, e o Método Analítico.
Segue abaixo o Script, e o gráfico:

```
clear all
clc
A = [-4,1;4,-4];
h = 0.05;
x0 = [100;0];
t = 5;
i = 1;
for j = 0:h:t
    x(:,i) = expm(A*j)*x0;
    tempo(i) = j;
    i = i+1;
end
x;
Analitico=x(1,:)'
tempo';
plot(tempo,Analitico)
hold on
clear all
h = 0.05;
tspan = [0,5];
y0 = [100;0];
[t,y] = euler_expl('Exercicio_3_btr',tspan,y0,h);
tempo = t
Euler = y(:,1)
plot(tempo,Euler)
clear all
h = 0.05;
tspan = [0,5];
y0 = [100;0];
[t,y] = rk4('Exercicio_3_btr',tspan,y0,h);
tempo = t
Ruge_Kutta = y(:,1)
plot(tempo,Ruge_Kutta)
xlabel('h')
ylabel('Mol/m³')
legend('Analitico','Euler','Ruge_Kutta')
```



Como podemos Analisar, o Método de Ruge-Kutta, é o método que mais se aproxima do Método Analítico. Isso é devido, o método de Ruge Kutta, ser realizado em diversos estágios.

4) exercício 5.5, p.355

5.5 In the study of fermentation kinetics, the logistic law

$$\frac{dy_1}{dt} = k_1 y_1 \left(1 - \frac{y_1}{k_2}\right)$$

has been used frequently to describe the dynamics of cell growth. This equation is a modification of the logarithmic law

$$\frac{dy_1}{dt} = k_1 y_1$$

The term $(1 - y_1/k_2)$ in the logistic law accounts for cessation of growth due to a limiting nutrient.

The logistic law has been used successfully in modeling the growth of *penicillium chryscogenum*, a penicillin-producing organism [6]. In addition, the rate of production of penicillin has been mathematically quantified by the equation

$$\frac{dy_2}{dt} = k_3 y_1 - k_4 y_2$$

Penicillin (y_2) is produced at a rate proportional to the concentration of the cell (y_1) and is degraded by hydrolysis, which is proportional to the concentration of the penicillin itself.

(a) Discuss other possible interpretations of the logistic law.
(b) Show that k_2 is equivalent to the maximum cell concentration that can be reached under given conditions.
(c) Apply the fourth-order Runge-Kutta integration method to find the numerical solution of the cell and penicillin equations. Use the following constants and initial conditions:

$k_1 = 0.03120$ $\quad k_2 = 47.70$ $\quad k_3 = 3.374$ $\quad k_4 = 0.01268$

at $t = 0$, $y_1(0) = 5.0$, and $y_2(0) = 0.0$; the range of t is $0 \le t \le 212$ h.

Se a concentração de y1 é máxima, dy1/dt = 0

$$\frac{dy1}{dt} = k1 * y1 * \left(1 - \frac{y1}{k2}\right) = 0$$

$$k1 * y1 = k1 * y1 * (\frac{y1}{k2})$$

$$1 = (\frac{y1}{k2})$$

$$y1_{max} = k2$$

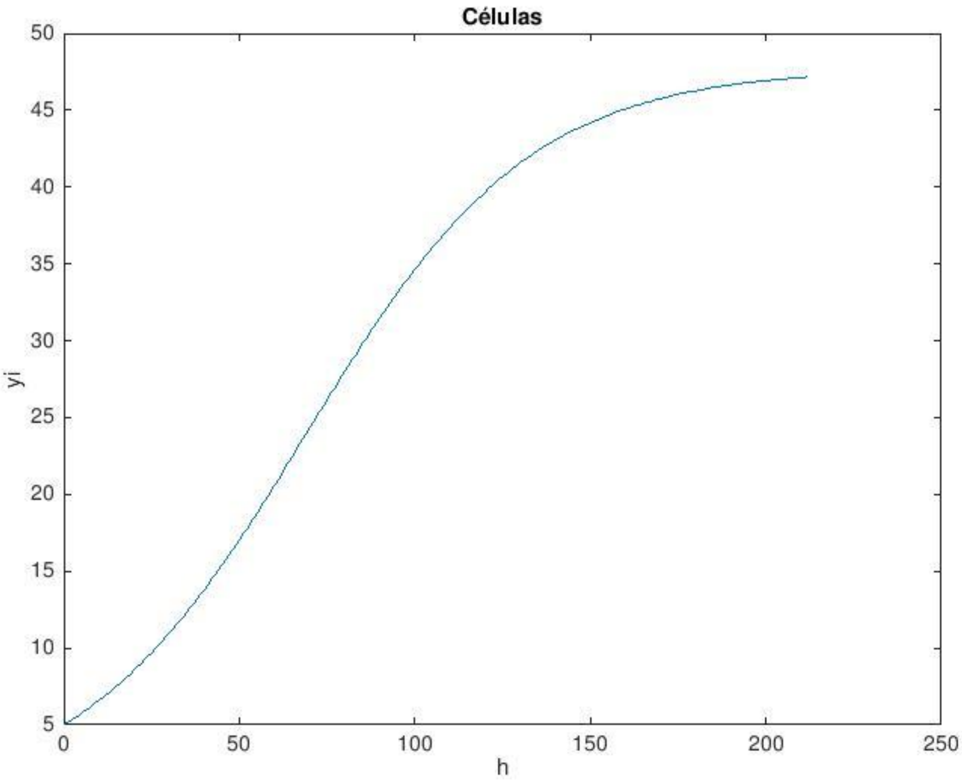
Iremos escrever uma função que descreve as reações acima:

```
function f = Exercicio_4_fermentacao(t,y)
    f = zeros(2,1);
    k1 = 0.0312;
    k2 = 47.7;
    k3 = 3.374;
    k4 = 0.01268;
f(1,1) = k1*y(1,1)-(k1*(y(1,1)^2))/k2;
    f(2,1) = k3*y(1,1)-k4*y(2,1);
end
```

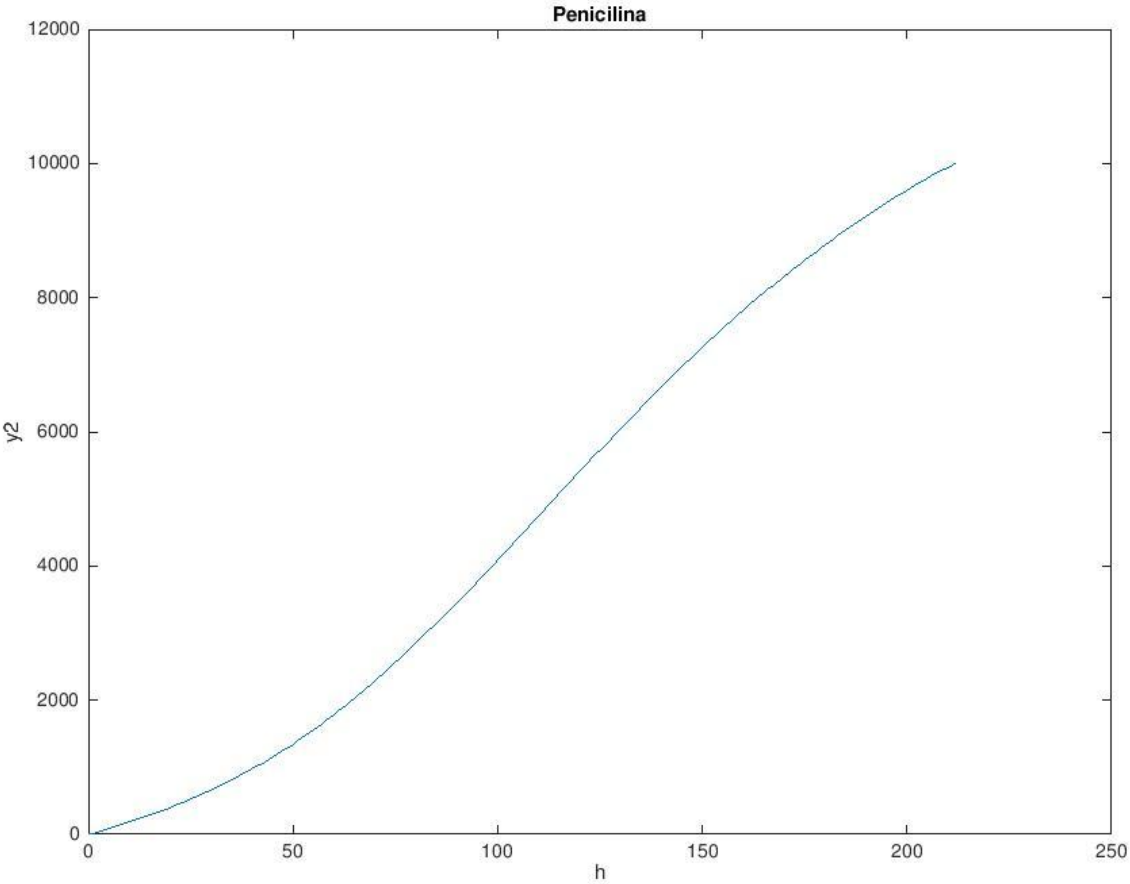
Aplicando o Método de Runge-Kutta de Quarta Ordem:

```
clear all
clc
h = 1;
tspan = [0,212];
y0 = [5;0];
[t,y] = rk4('Exercicio_4_fermentacao',tspan,y0,h);
y1 = y(:,1)
y2 = y(:,2)
tempo = t
plot(tempo,y1)
hold on
plot(tempo,y2)
xlabel('h')
ylabel('yi')
legend('y1','y2')
```

Podemos Plotar os seguintes Gráficos:



Células
yi
h
50
45
40
35
30
25
20
15
10
5
0
50
100
150
200
250


Penicilina
12000
10000
8000
6000
4000
2000
0
y2
0
50
100
150
200
250
h

5) exercício 5.6, p.356

5.6 The conversion of glucose to gluconic acid is a simple oxidation of the aldehyde group of the sugar to a carboxyl group. This transformation can be achieved by a microorganism in a fermentation process. The enzyme glucose oxidase, present in the microorganism, converts glucose to gluconolactone. In turn, the gluconolactone hydrolyzes to form the gluconic acid. The overall mechanism of the fermentation process that performs this transformation can be described as follows:

Cell growth:

$$\text{Glucose} + \text{Cells} \rightarrow \text{Cells}$$

Glucose oxidation:

$$\text{Glucose} + O_2 \xrightarrow{\text{Glucose oxidase}} \text{Gluconolactone} + H_2O_2$$

Gluconolactone hydrolysis:

$$\text{Gluconolactone} + H_2O \longrightarrow \text{Gluconic acid}$$

Peroxide decomposition:

$$H_2O_2 \xrightarrow{\text{Catalyst}} H_2O + \frac{1}{2}O_2$$

A mathematical model of the fermentation of the bacterium *Pseudomonas ovalis*, which produces gluconic acid, has been developed by Rai and Constantinides [10]. This model, which describes the dynamics of the logarithmic growth phases, can be summarized as follows:

Rate of cell growth:

$$\frac{dy_1}{dt} = b_1 y_1 \left(1 - \frac{y_1}{b_2}\right)$$

Rate of gluconolactone formation:

$$\frac{dy_2}{dt} = \frac{b_3 y_1 y_4}{b_4 + y_4} - 0.9082 b_5 y_2$$

Rate of gluconic acid formation:

$$\frac{dy_3}{dt} = b_5 y_2$$

Rate of glucose consumption:

$$\frac{dy_4}{dt} = -1.011\left(\frac{b_3 y_1 y_4}{b_4 + y_4}\right)$$

where y_1 = concentration of cell
y_2 = concentration of glucononctone
y_3 = concentration of gluconic acid
y_4 = concentration of glucose
b_1-b_5 = parameters of the system which are functions of temperature and pH.

At the operating conditions of 30°C and pH 6.6, the values of the five parameters were determined from experimental data to be

$b_1 = 0.949 \quad b_2 = 3.439 \quad b_3 = 18.72 \quad b_4 = 37.51 \quad b_5 = 1.169$

At these conditions, develop the time profiles of all variables, y_1 to y_4, for the period $0 \le t \le 9$ h. The initial conditions at the start of this period are

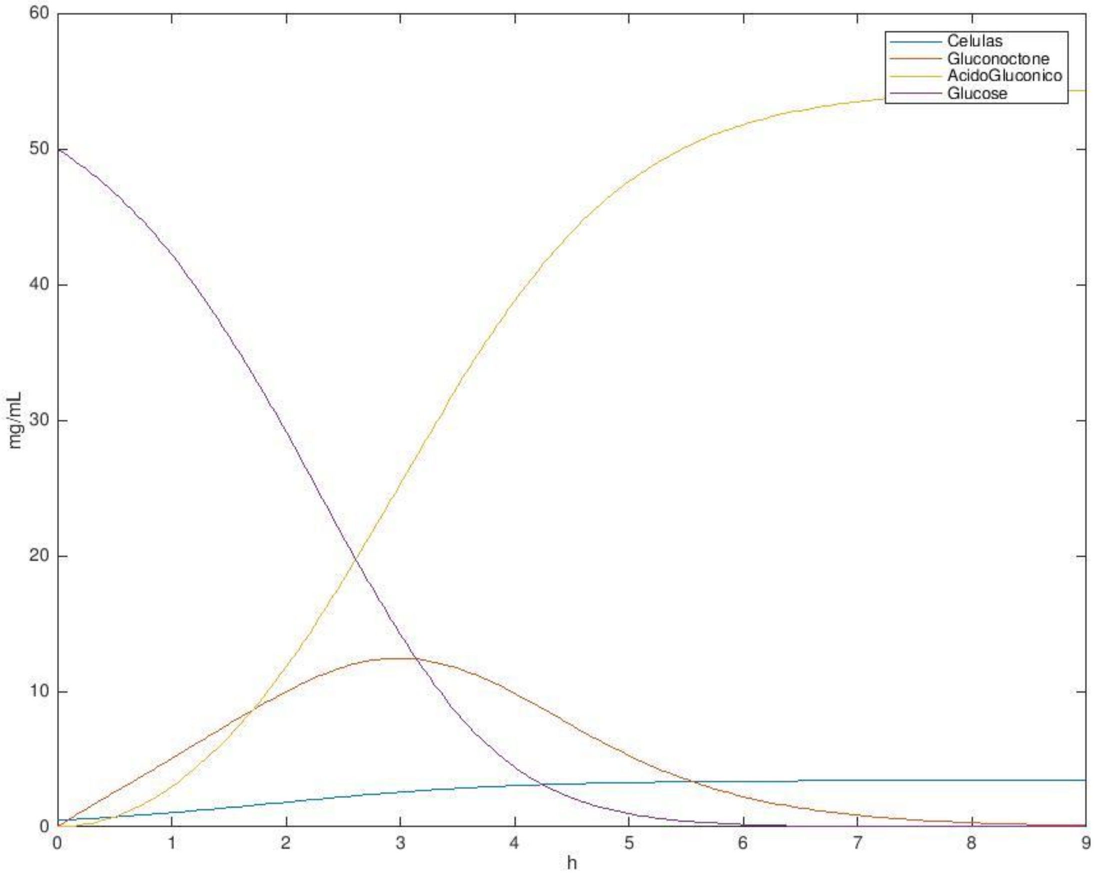
$y_1(0) = 0.5$ U.O.D./mL $\quad y_3(0) = 0.0$ mg/mL
$y_2(0) = 0.0$ mg/mL $\quad y_4(0) = 50.0$ mg/mL

Iremos escrever uma função para os balanços acima:

```
function f = Exercicio_5_6_glucose(t,y)
    b1 = 0.949;
    b2 = 3.439;
    b3 = 18.72;
    b4 = 37.51;
    b5 = 1.169;
f = zeros(4,1);
    f(1,1) = b1*y(1,1)*(1-(y(1,1)/b2));
f(2,1) = ((b3*y(1,1)*y(4,1))/(b4+y(4,1)))-0.9082*b5*y(2,1);
    f(3,1) = b5*y(2,1);
f(4,1) = -1.011*((b3*y(1,1)*y(4,1))/(b4+y(4,1)))
end
```

Iremos escrever um Script para a plotagem dos Gráficos e aplicando o método de Runge-Kutta, devido sua maior precisão:

```
clear all
clc
h = 0.05;
tspan = [0,9];
y0 = [0.5;0;0;50];
[t,y] = rk4('Exercicio_5_6_glucose',tspan,y0,h);
Celulas = y(:,1)
Gluconoctone = y(:,2)
AcidoGluconico = y(:,3)
Glucose = y(:,4)
tempo = t
plot(tempo,Celulas)
hold on
plot(tempo,Gluconoctone)
plot (tempo,AcidoGluconico)
plot(tempo,Glucose)
xlabel('h')
ylabel('mg/mL')
legend('Celulas','Gluconoctone','AcidoGluconico','Glucose')
```



6) exercício 5.10, p.363

5.10 A plug-flow reactor is to be designed to produce the product D from A according to the following reaction:

$$A \rightarrow D \qquad r_D = 60C_A \text{ mole } D\,/\,\text{L.s}$$

In the operating condition of this reactor, the following undesired reaction also takes place:

$$A \rightarrow U \qquad r_U = \frac{0.003C_A}{1 + 10^5 C_A} \text{ mole } U\,/\,\text{L.s}$$

The undesired product U is a pollutant and it costs 10 \$/mol U to dispose it, whereas the desired product D has a value of 35 \$/mol D. What size of reactor should be chosen in order to obtain an effluent stream at its maximum value?

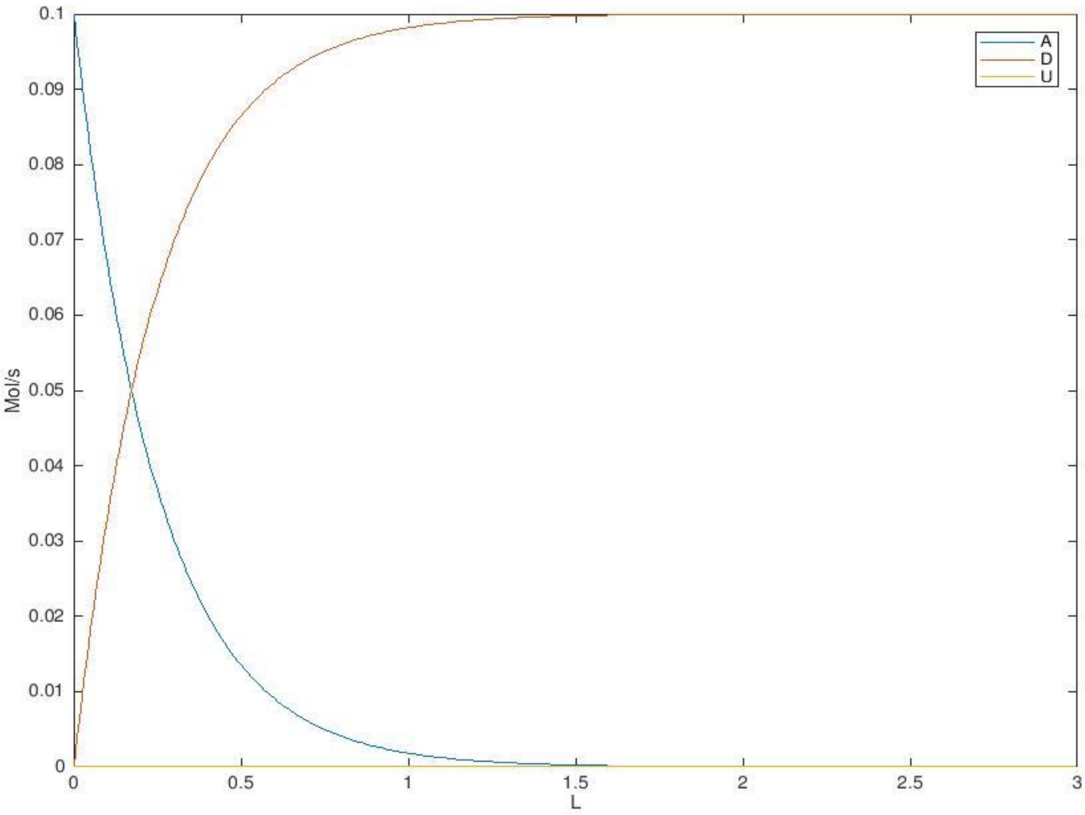
Pure reactant A with volumetric flow rate of 15 L/s and molar flow rate of 0.1 mol/s enters the reactor. Value of A is 5 \$/mol A.

Iremos Escrever uma função para o cálculo das concentrações de A,D e U em função do volume do reator

```
function f = Exercicio_6_pfr(V,y)
    f = zeros(3,1);
rd = 60*(y(1,1)/15);
    ru = (0.003*(y(1,1)/15))/(1+1e5*(y(1,1)/15));
    f(1,1) = -rd -ru;
f(2,1) = rd;
    f(3,1) = ru;
end
```

Escrevendo um Script para analisarmos as concentrações dos 3 componentes em relação ao volume:

```
clear all
clc
tspan = [0,3]; % Chute inicial de estudo do Volume
y0 = [0.1;0;0]; %Fa0
h = 0.01;
[t,y]  = rk4('Exercicio_6_pfr',tspan,y0,h);
A = y(:,1)
D = y(:,2)
U = y(:,3)
volume = t;
plot(volume,A)
hold on
plot(volume,D)
plot(volume,U)
xlabel('L')
ylabel('Mol/s')
legend('A','D','U')
```



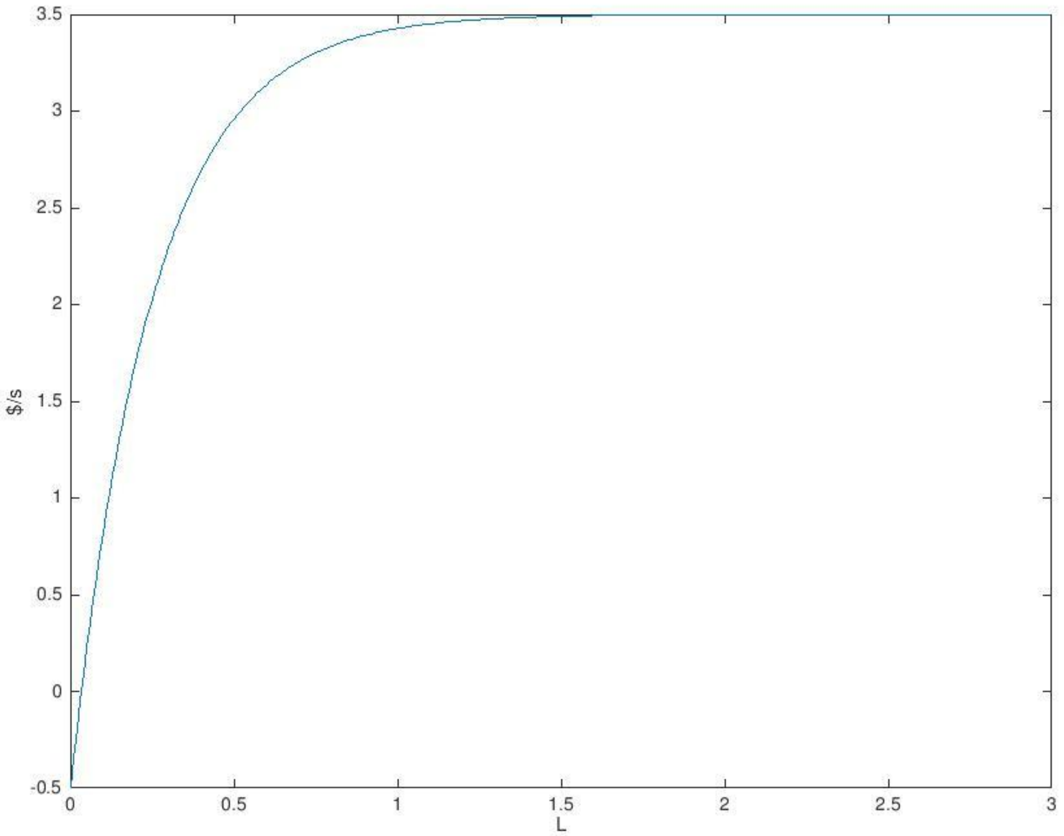
Como podemos analisar no gráfico acima, U não é produzido, e a partir do momento que A não é todo consumido, é encerrado a produção de D

O Lucro será:

$$Lucro = C_D * 35 - C_A * 5 - C_U * 10$$

Escrevendo o Script para plotarmos o lucro em função do volume do reator:

```
clear all
clc
tspan = [0,3]; % Chute inicial de estudo do Volume
y0 = [0.1;0;0]; %Fa0
h = 0.01;
[t,y]  = rk4('Exercicio_6_pfr',tspan,y0,h);
A = y(:,1);
D = y(:,2);
U = y(:,3);
volume = t;
lucro = D*35-A*5-U*10
plot(volume,lucro)
xlabel('L');
ylabel('$/s')
```



Analisando o gráfico, o lucro máximo será com um reator de 1,5 L

7) exemplo 6.1 (a) e (b), p.382

Example 6.1: Solution of the Laplace and Poisson Equations. Write a general MATLAB function to determine the numerical solution of a two-dimensional elliptic partial differential equation of the general form:

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = f$$

for a rectangular object of variable width and height. The object could have Dirichlet, Neumann, or Robbins boundary conditions. The value of f should be assumed to be a constant. Use this function to find the solution of the following problems ($u = T$):

(*a*) A thin square metal plate of dimensions 1 m × 1 m is subjected to four heat sources which maintain the temperature on its four edges as follows:

$$T(0, y) = 250°\text{C}$$

$$T(1, y) = 100°\text{C}$$

$$T(x, 0) = 500°\text{C}$$

$$T(x, 1) = 25°\text{C}$$

The flat sides of the plate are insulated so that no heat is transferred through these sides. Calculate the temperature profiles within the plate.

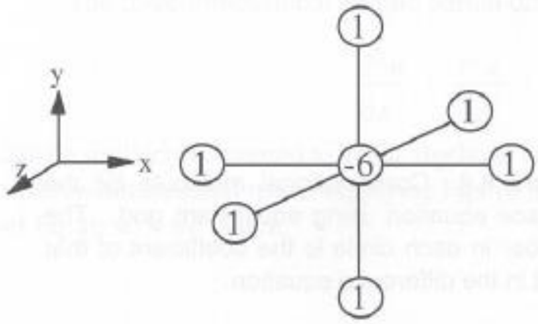


Figure 6.5 Computational molecule for the three-dimensional elliptic differential equation using equidistant grid.

(*b*) Perfect insulation is installed on two edges (right and top) of the plate of part (*a*). The other two edges are maintained at constant temperatures. The set of Dirichlet and Neumann boundary conditions is

$$T(0, y) = 250^\circ C$$

$$\frac{\partial T}{\partial x}\Big|_{1,y} = 0$$

$$T(x, 0) = 500^\circ C$$

$$\frac{\partial T}{\partial x}\Big|_{x,1} = 0$$

Calculate the temperature profiles within the plate and compare these with the results of part (*a*).

Iremos aproximar as derivadas parciais segundas em diferenças finitas centrais:

Considerando o passo Δx e Δy como h, pois iremos dividir os duas dimensões (x,y) em passos iguais. Sendo U=T

$$\frac{\partial^2 u}{\partial x^2} = \frac{T_{i+1,j} - 2 * T_{i,j} + T_{i-1,j}}{h^2}$$

$$\frac{\partial^2 u}{\partial y^2} = \frac{T_{i,j+1} - 2 * T_{i,j} + T_{i,j-1}}{h^2}$$

$$\frac{T_{i+1,j} - 2 * T_{i,j} + T_{i-1,j}}{h^2} + \frac{T_{i,j+1} - 2 * T_{i,j} + T_{i,j-1}}{h^2} = f$$

$$T_{i-1,j} + T_{i+1,j} - 4 * T_{i,j} + T_{i,j-1} + T_{i,j+1} = f * h^2$$

a) Para o caso do item a:

C.C.1: $x = 0$ e $0 \leq y \leq 1$ $T = 250°C$ -> $T(0,j) = 250$

C.C.2: $x = 1$ e $0 \leq y \leq 1$ $T = 100°C$ -> $T(N,j) = 100$

C.C.3: $0 \leq x \leq 1$ e $y = 0$ $T = 500°C$ -> $T(i,0) = 500$

C.C.4: $0 \leq x \leq 1$ e $y = 1$ $T = 25°C$ -> $T(i,N) = 25$

Como temos 4 condiçoes de contorno (2 para cada dimensão), o numero de incógnitas é (N-1)*(N-1) = (N-1)^2, onde N, é o número de divisões

Logo, iremos realizar o balanço para as seguintes condições:

Se j = 1 e i = 1

$$T_{0,1} + T_{2,1} - 4 * T_{1,1} + T_{1,0} + T_{1,2} = f * h^2$$

$$T_{2,1} - 4 * T_{1,1} + T_{1,2} = f * h^2 - T_{0,1} - T_{1,0}$$

Se j = 1 e i < (N-1)

$$T_{i-1,j} + T_{i+1,j} - 4 * T_{i,1} + T_{i,0} + T_{i,2} = f * h^2$$

$$T_{i-1,1} + T_{i+1,1} - 4 * T_{i,1} + T_{i,2} = f * h^2 - T_{i,0}$$

Se j = 1 e i = (N-1)

$$T_{N-2,1} + T_{N,1} - 4 * T_{N-1,1} + T_{N-1,0} + T_{N-1,2} = f * h^2$$

$$T_{N-2,1} - 4 * T_{N-1,1} + T_{N-1,2} = f * h^2 - T_{N,1} - T_{N-1,0}$$

Se j < (N-1) e i = 1

$$T_{0,j} + T_{2,j} - 4 * T_{1,j} + T_{1,j-1} + T_{1,j+1} = f * h^2$$

$$T_{2,j} - 4 * T_{1,j} + T_{1,j-1} + T_{1,j+1} = f * h^2 - T_{0,j}$$

Se j < (N-1) e i < (N-1)

$$T_{i-1,j} + T_{i+1,j} - 4 * T_{i,j} + T_{i,j-1} + T_{i,j+1} = f * h^2$$

Se j<(N-1) e i = (N-1)

$$T_{N-2,j} + T_{N,j} - 4 * T_{N-1,j} + T_{N-1,j-1} + T_{N-1,j+1} = f * h^2$$

$$T_{N-2,j} - 4 * T_{N-1,j} + T_{N-1,j-1} + T_{N-1,j+1} = f * h^2 - T_{N,j}$$

Se j=(N-1) e i = 1

$$T_{0,N-1} + T_{2,N-1} - 4 * T_{1,N-1} + T_{1,N-2} + T_{1,N} = f * h^2$$

$$T_{2,N-1} - 4 * T_{1,N-1} + T_{1,N-2} = f * h^2 - T_{1,N} - T_{0,N-1}$$

Se j = (N-1) e i < (N-1)

$$T_{i-1,N-1} + T_{i+1,N-1} - 4 * T_{i,N-1} + T_{i,N-2} + T_{i,N} = f * h^2$$

$$T_{i-1,N-1} + T_{i+1,N-1} - 4 * T_{i,N-1} + T_{i,N-2} = f * h^2 - T_{i,N}$$

Se j = (N-1) e i = (N-1)

$$T_{N-2,N-1} + T_{N,N-1} - 4 * T_{N-1,N-1} + T_{N-1,N-2} + T_{N-1,N} = f * h^2$$

$$T_{N-2,N-1} - 4 * T_{N-1,N-1} + T_{N-1,N-2} = f * h^2 - T_{N,N-1} - T_{N-1,N}$$

b) Para o caso do item b:

C.C.1: x = 0 e $0 \leq y \leq 1$ T = 250°C -> T(0,j) = 250

C.C.2: x =1 e $0 \leq y \leq 1$ dT/dx = 0

C.C.3: $0 \leq x \leq 1$ e y = 0 T = 500°C -> T(i,0) = 500

C.C.4: $0 \leq x \leq 1$ e y = 1 dT/dy = 0

Como temos 2 condições de contorno (1 para cada dimensão), o número de incógnitas é (N)*(N) = (N)^2, onde N, é o número de divisões

Realizando aproximação por diferencial central:

$$\frac{dT}{dx} = \frac{T_{i+1,j} - T_{i-1,j}}{2 * h} = 0$$

$$T_{i+1,j} = T_{i-1,j}$$

$$\frac{dT}{dy} = \frac{T_{i,j+1} - T_{i,j-1}}{2 * h} = 0$$

$$T_{i,j+1} = T_{i,j-1}$$

Logo, iremos realizar o balanço para as seguintes condições:

Se j = 1 e i = 1

$$T_{0,1} + T_{2,1} - 4 * T_{1,1} + T_{1,0} + T_{1,2} = f * h^2$$

$$T_{2,1} - 4 * T_{1,1} + T_{1,2} = f * h^2 - T_{0,1} - T_{1,0}$$

Se j = 1 e i < (N)

$$T_{i-1,j} + T_{i+1,j} - 4 * T_{i,1} + T_{i,0} + T_{i,2} = f * h^2$$

$$T_{i-1,j} + T_{i+1,j} - 4 * T_{i,1} + T_{i,2} = f * h^2 - T_{i,0}$$

Se j = 1 e i = (N)

$$T_{N-1,1} + T_{N+1,1} - 4 * T_{N,1} + T_{N,0} + T_{N,2} = f * h^2$$

Como

$$T_{i+1,j} = T_{i-1,j}$$

$$2 * T_{N-1,1} - 4 * T_{N,1} + T_{N,0} + T_{N,2} = f * h^2$$

$$2 * T_{N-1,1} - 4 * T_{N,1} + T_{N,2} = f * h^2 - T_{N,0}$$

Se j < (N) e i = 1

$$T_{0,j} + T_{2,j} - 4 * T_{1,j} + T_{1,j-1} + T_{1,j+1} = f * h^2$$

$$T_{2,j} - 4 * T_{1,j} + T_{1,j-1} + T_{1,j+1} = f * h^2 - T_{0,j}$$

Se j < (N) e i < (N)

$$T_{i-1,j} + T_{i+1,j} - 4 * T_{i,j} + T_{i,j-1} + T_{i,j+1} = f * h^2$$

Se j<(N) e i = (N)

$$T_{N-1,j} + T_{N+1,j} - 4 * T_{N,j} + T_{N,j-1} + T_{N,j+1} = f * h^2$$

Como

$$T_{i+1,j} = T_{i-1,j}$$

$$2 * T_{N-1,j} - 4 * T_{N,j} + T_{N,j-1} + T_{N,j+1} = f * h^2$$

Se j=(N) e i = 1

$$T_{0,N} + T_{2,N} - 4 * T_{1,N} + T_{1,N-1} + T_{1,N+1} = f * h^2$$

como

$$T_{i,j+1} = T_{i,j-1}$$

$$T_{0,N} + T_{2,N} - 4 * T_{1,N} + 2 * T_{1,N-1} = f * h^2$$

$$T_{2,N} - 4 * T_{1,N} + 2 * T_{1,N-1} = f * h^2 - T_{0,N}$$

Se j = (N) e i < (N)

$$T_{i-1,N} + T_{i+1,N} - 4 * T_{i,N} + T_{i,N-1} + T_{i,N+1} = f * h^2$$

como

$$T_{i,j+1} = T_{i,j-1}$$

$$T_{i-1,N} + T_{i+1,N} - 4 * T_{i,N} + 2 * T_{i,N-1} = f * h^2$$

Se j = (N) e i = (N)

$$T_{N-1,N} + T_{N+1,N} - 4 * T_{N,N} + T_{N,N-1} + T_{N,N+1} = f * h^2$$

como

$$T_{i,j+1} = T_{i,j-1}$$

e

$$T_{i+1,j} = T_{i-1,j}$$

$$2 * T_{N-1,N} - 4 * T_{N,N} + 2 * T_{N,N-1} = f * h^2$$