Prof. Davide Manca – Politecnico di Milano

**Dynamics and Control of Chemical Processes**

## Solution to Lab #1

# Introduction to System Dynamics

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# E1 – Dynamics of a biological system

A biological process is run in a batch reactor where the biomass (B) grows by feeding on the substrate (S). The material balances for the two species are:

$$\begin{cases} \dfrac{dB}{dt} = \dfrac{k_1 BS}{k_2 + S} \\ \dfrac{dS}{dt} = -k_3 \dfrac{k_1 BS}{k_2 + S} \end{cases}$$

With: $k_1 = 0.5\ \mathrm{h}^{-1}$ $\quad k_2 = 10^{-7}\ \mathrm{kmol/m^3}$ $\quad k_3 = 0.6$

The initial conditions are:

$$\begin{cases} B(0) = 0.03\ \ \mathrm{kmol/m^3} \\ S(0) = 4.5\ \ \mathrm{kmol/m^3} \end{cases}$$

# E1 - Aim

- Determine the dynamic evolution of both biomass and substrate over a time interval of 15 h.

- Use Matlab to solve the ordinary differential equations (ODE) system: (i) with the standard precision (*i.e.* by default) for both absolute and relative tolerances. (ii) Modify those tolerances with a relative tolerance of **`1.e-8`** and an absolute one of **`1.e-12`**. Compare the two dynamics and provide a comment about them.

# Integration of ODE in MATLAB

To integrate the ordinary differential system one can use the functions implemented in MATLAB:

**ode15s**: for the integration of stiff systems

```
[t,y] = ode15s(@(t,y)myFun(t,y,params),tSpan,y0,options)
```

**ode45**: for the integration of non-stiff systems.

```
[t,y] = ode45(@(t,y)myFun(t,y,params),tSpan,y0,options)
```

# Integration of ODE in MATLAB

- Where:
  - `t` = time
  - `y` = the dependent variables matrix (each column represents a variable)
  - `myFun` = name of the ODE function
  - `tSpan` = integration time span `[tMin tMax]`
  - `y0` = vector of initial conditions, *e.g.*, `[B0 S0]`
  - `params` = list of optional parameters for the solution of the differential system (*e.g.*, $k_1$, $k_2$, $k_3$) [`params` vector must however be always present even if no specific parameters are used)
  - `options` = options for the integrator

```
options = odeset('RelTol',1E-8,'AbsTol',1E-12)
```

# MATLAB code

## Main

```
k1 = 0.5;               % [h-1]
k2 = 1E-7;              % [kmol]
k3 = 0.6;               % [-]
tSpan = [0 15];         % [h]
y0 = [0.03 4.5];        % [kmol] y0(1) = B; y0(2) = S
options = odeset('RelTol',1E-8,'AbsTol',1E-12);
[t,y] = ode45(@(t,y)Sisdif(t,y,k1,k2,k3),tSpan,y0,options);
B = y(:,1);
S = y(:,2);
```

# MATLAB code

## Sisdif

```
function dy = Sisdif(t,y,k1,k2,k3)
   dy = zeros(2,1); % column vector
   B = y(1);
   S = y(2);
   dy(1) = k1*B*S / (S + k2);
   dy(2) = - k3 * dy(1);
```

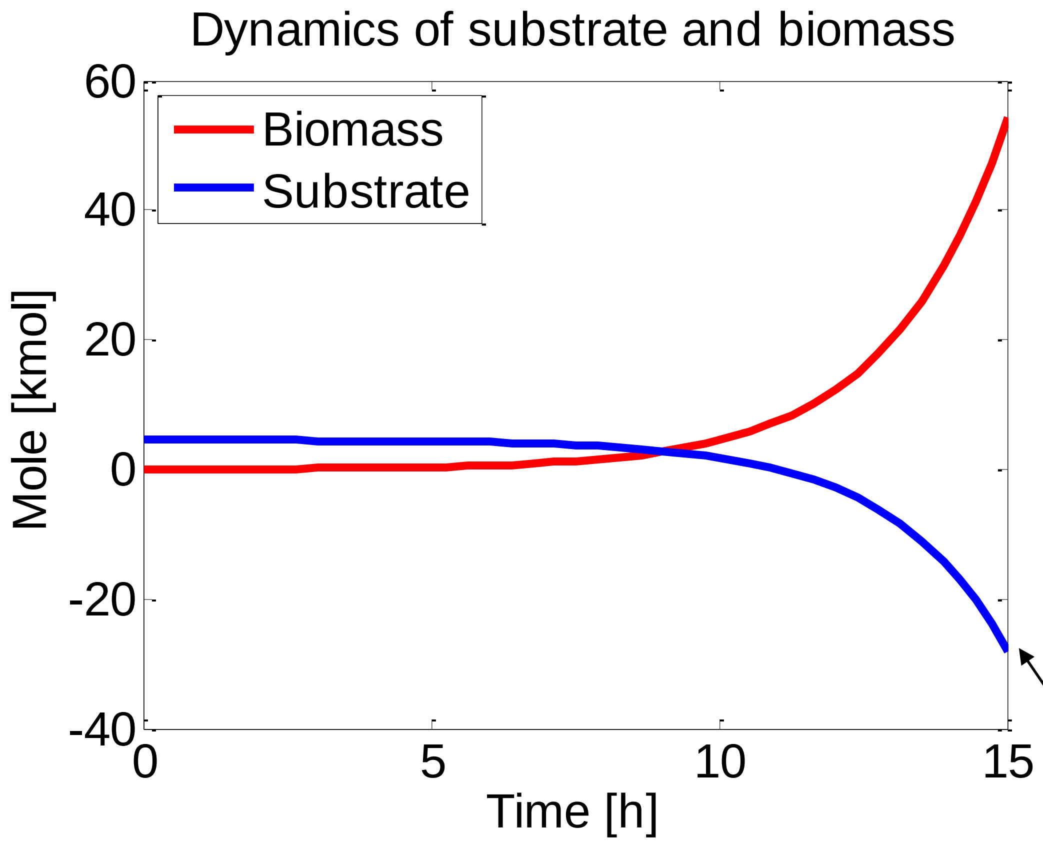
# MATLAB code

## Results display

```
figure(1)

plot(t,B,'r',t,S,'b','LineWidth',3)

set(gca,'FontSize',18)

legend('Biomass','Substrate',2)

xlabel('Time [h]')

ylabel('Mass [kmol]')

title('Dynamics of substrate and biomass')

grid off

saveas(figure(1),'Biological System.emf')
```

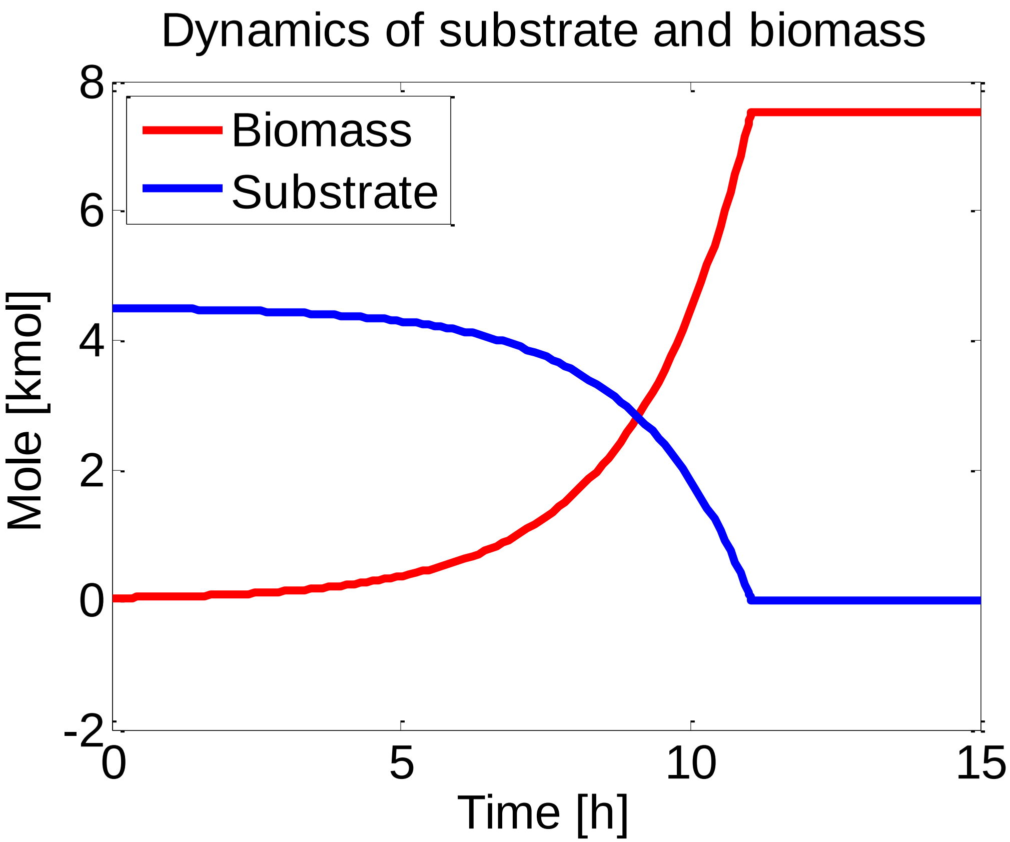
Advice: do not use the extension .fig

# Dynamics of a biological system (1)




Physically impossible

# Dynamics of a biological system (2)

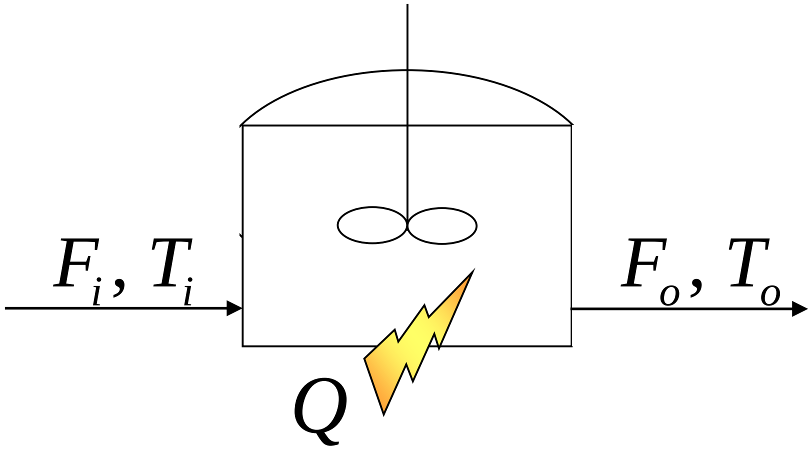


# E2 – Dynamics of a perfectly mixed tank

An intermediate tank is perfectly mixed (*i.e.* it is a continuously stirred tank, *aka* CST) and heated. Determine the dynamics of the outlet temperature when there is a step disturbance of 30 °C in the inlet temperature, with:

- Heating power: $Q = 1 \text{ MW}$
- Inlet flowrate: $F_i = 8 \text{ kmol/s}$
- CST mass holdup: $m = 100 \text{ kmol}$
- Specific molar heat: $cp = 2.5 \text{ kJ/kmol K}$
- Initial inlet temperature: $T_i = 300 \text{ K}$

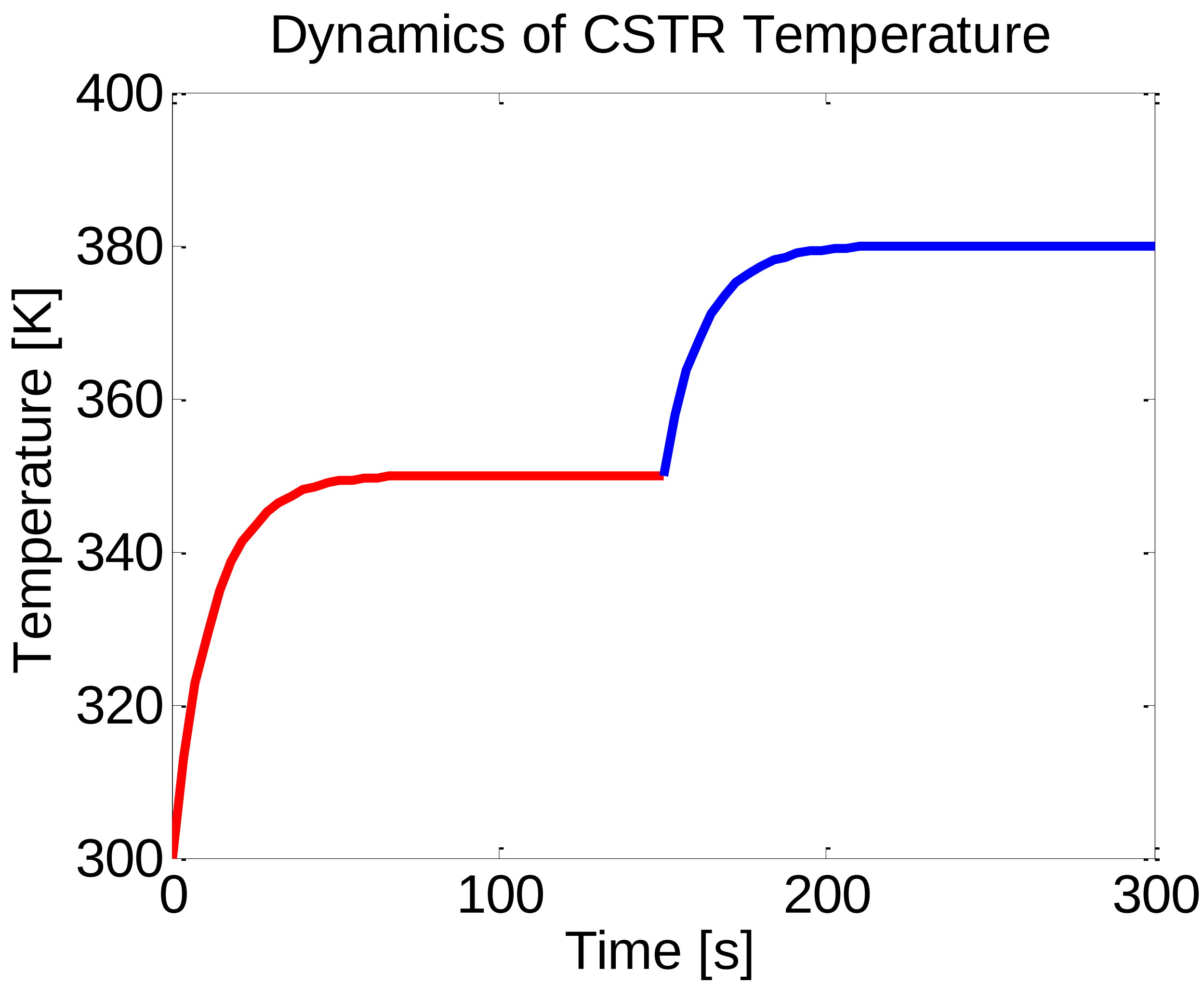
# Modelling of the system



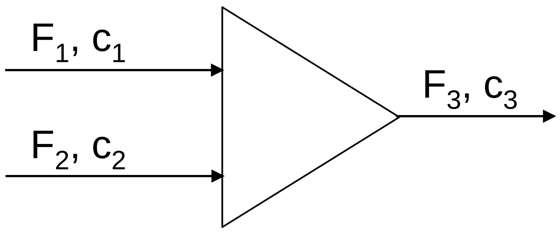

Mass balance: $$F_i = F_o$$

Energy balance: $$m c_p \frac{dT}{dt} = -F_o c_p \left(T_o - T_i\right) + Q$$

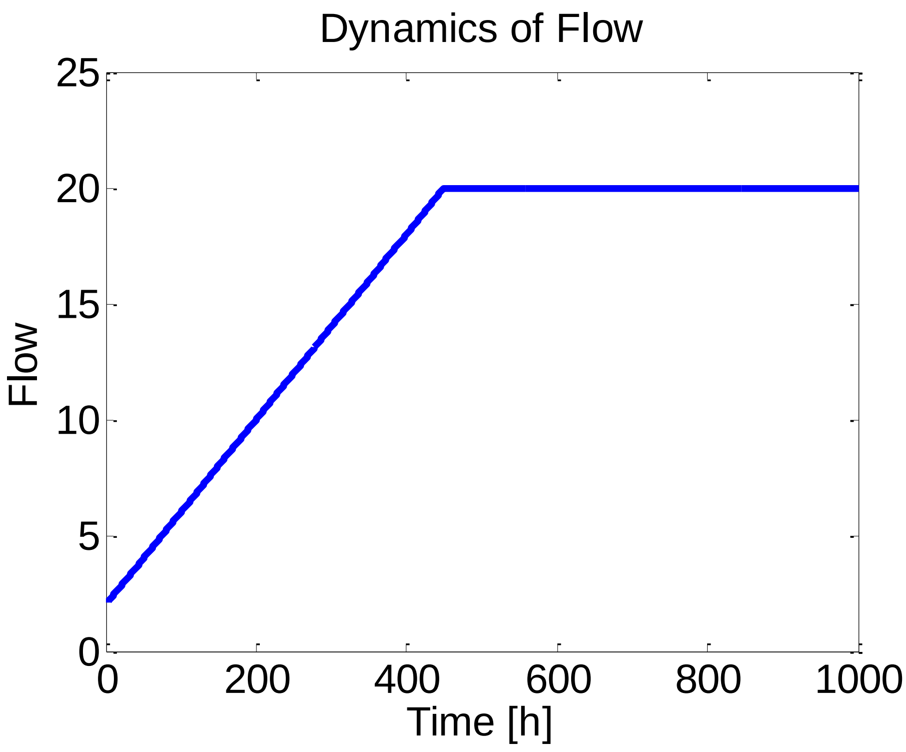
# Results


Dynamics of CSTR Temperature
400
380
360
340
320
300
0
100
200
300
Temperature [K]
Time [s]

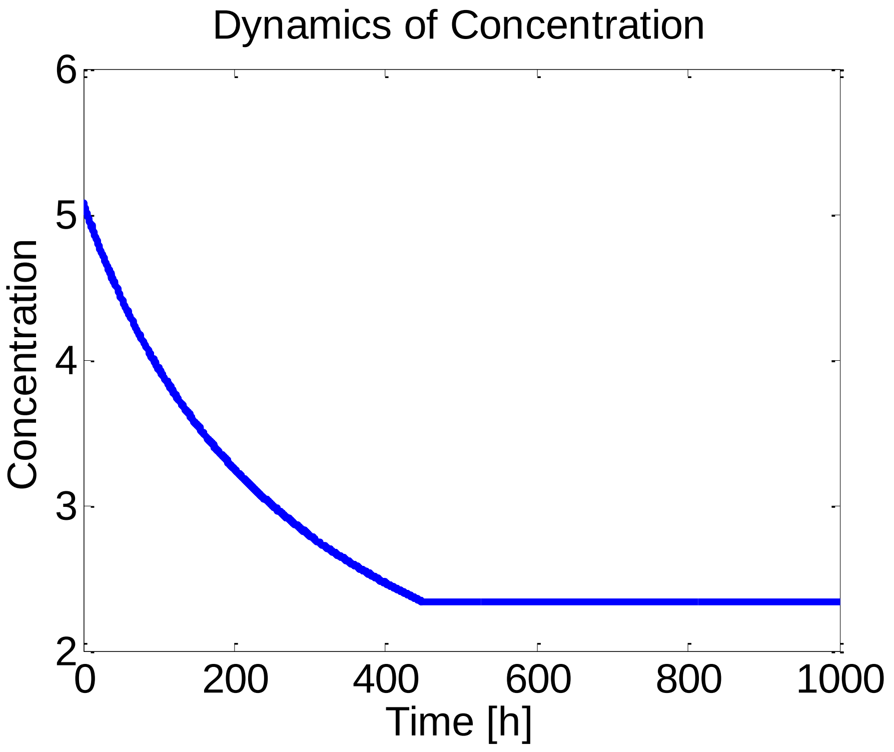
# E3 - Mixer



$F_1$, $c_1$
$F_2$, $c_2$
$F_3$, $c_3$

Dynamics of Flow
Flow
Time [h]
0
200
400
600
800
1000
5
10
15
20
25

Dynamics of Concentration
Concentration
Time [h]
0
200
400
600
800
1000
2
3
4
5
6

# E4 –Runaway dynamics