Matteo Pelucchi – Politecnico di Milano

Dynamics and Control of Chemical Processes

Solution to Practicals #1

Introduction to System Dynamics

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)
```

Default relative error tolerance 1.e-3 and the default absolute tolerance of 1.e-6.

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);
end
```

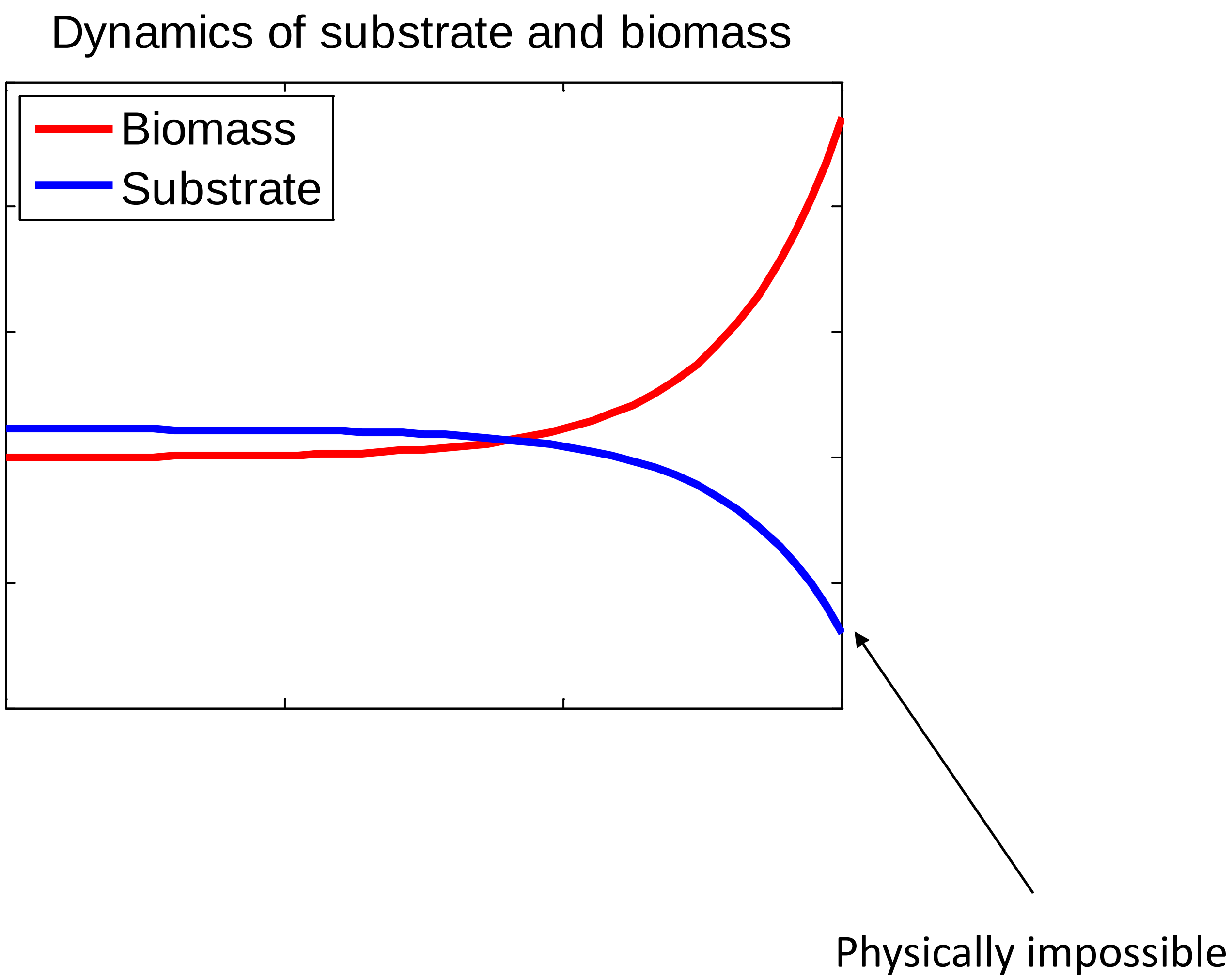
MATLAB code

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')
```

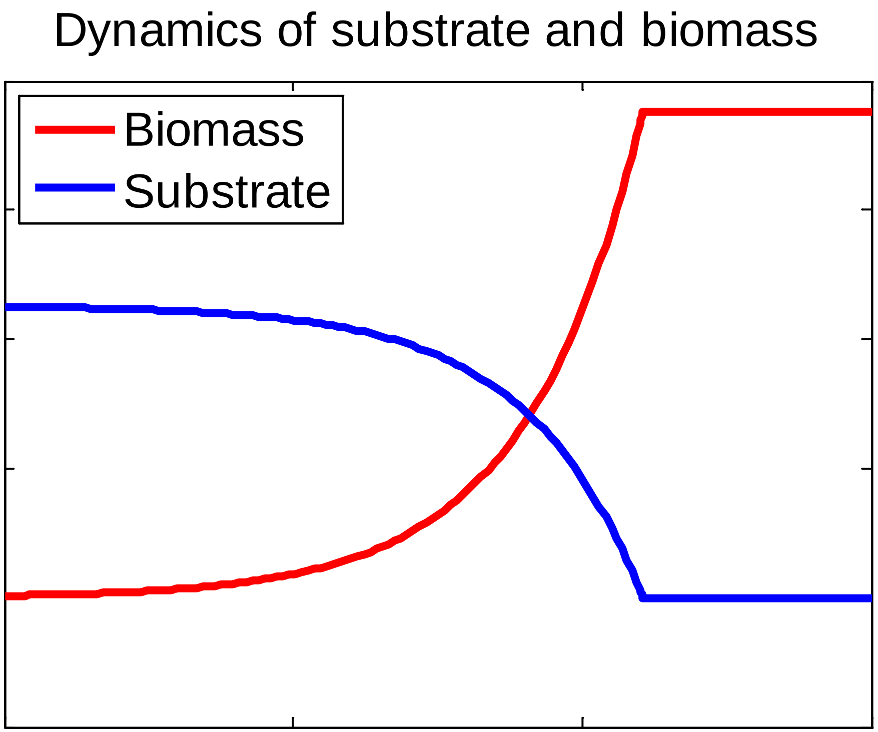
Dynamics of a biological system (1)

Default tolerances



Dynamics of a biological system (2)

Tighter tolerances

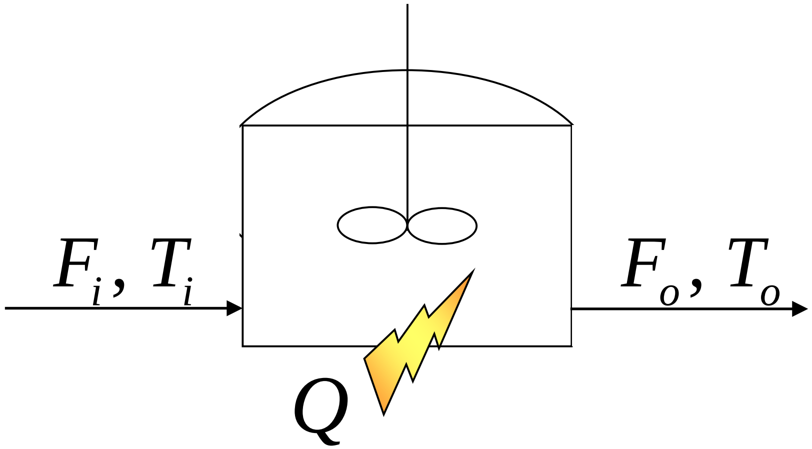


E2 – Dynamics of a perfectly mixed tank

An intermediate tank is perfectly mixed (*i.e.* it is a continuously stirred tank, *i.e.* 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: $T_i = 300 \text{ K}$

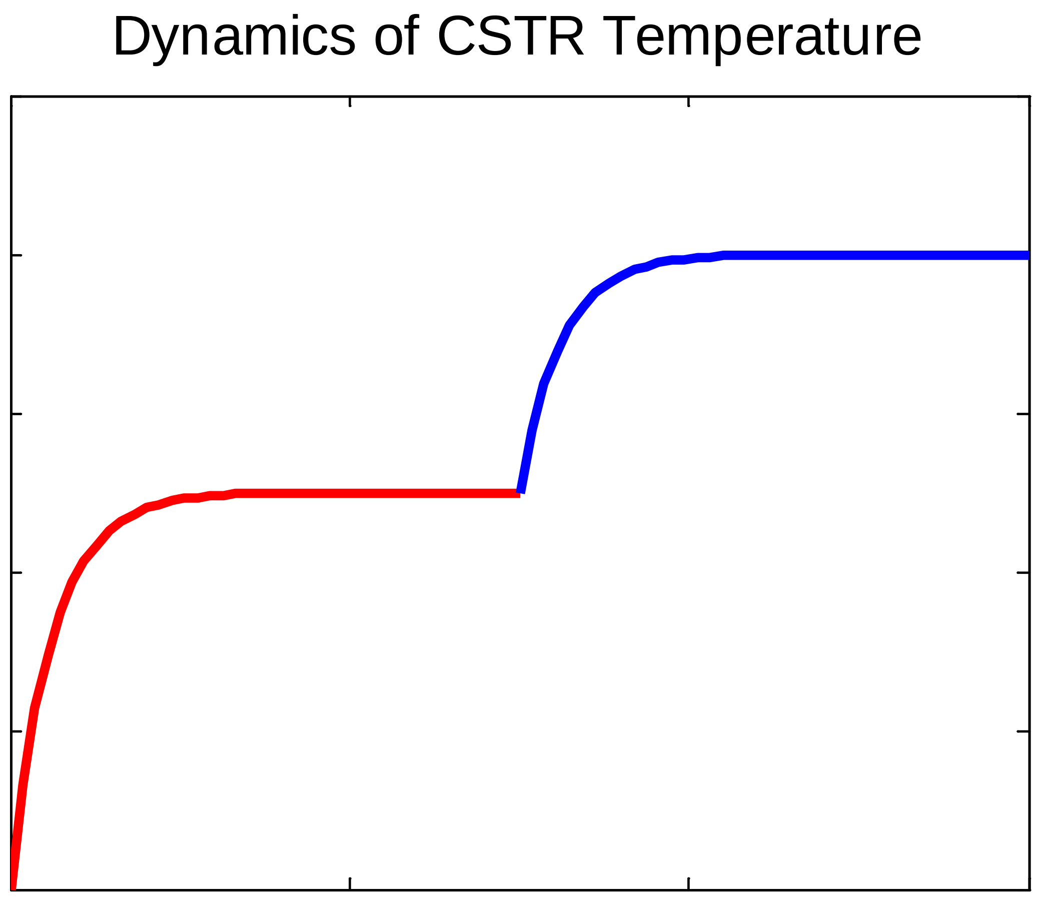
Modelling of the system



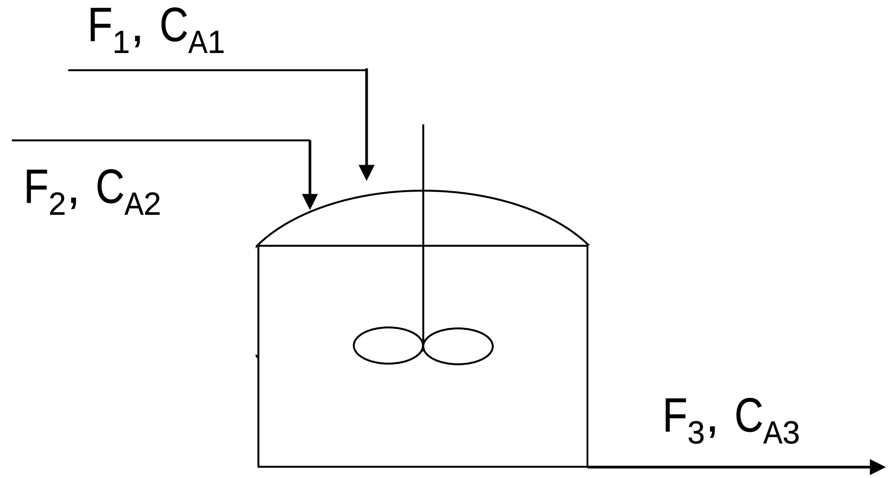
Mass balance: $F_i = F_o$

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

Results



E3 - Mixer



Total mass balance:

$$\rho \frac{dV}{dt} = (\rho_1 F_1 + \rho_2 F_2) - \rho_3 F_3 = 0$$

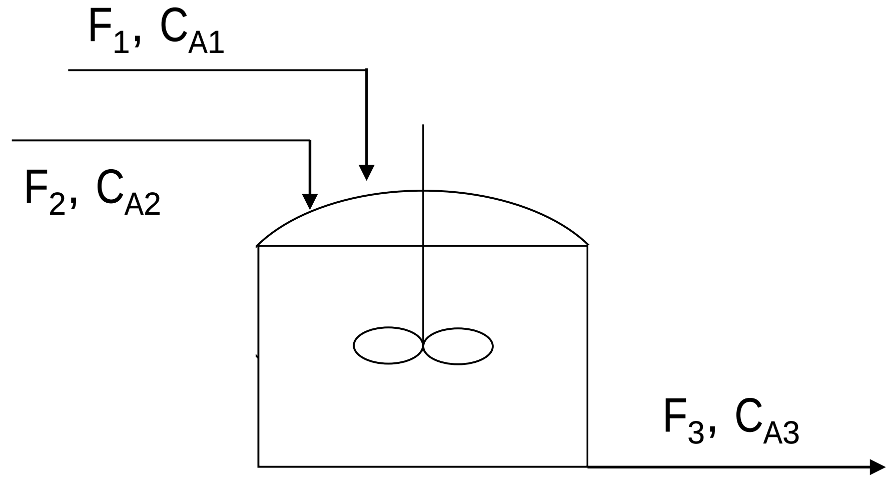
$$\rho = \rho_1 = \rho_2 = \rho_3$$

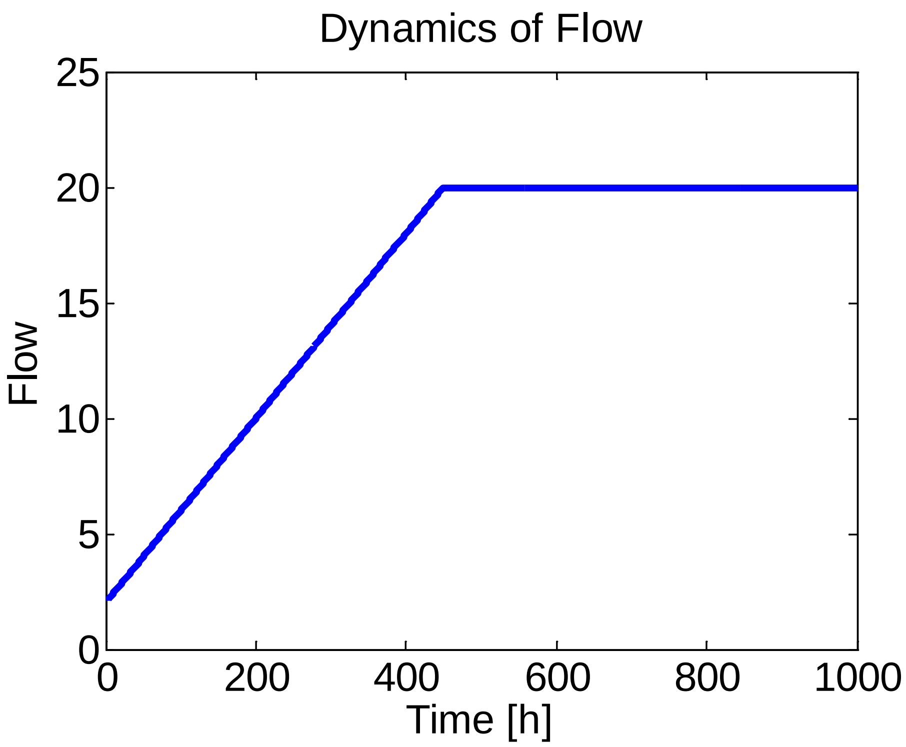
Component balance:

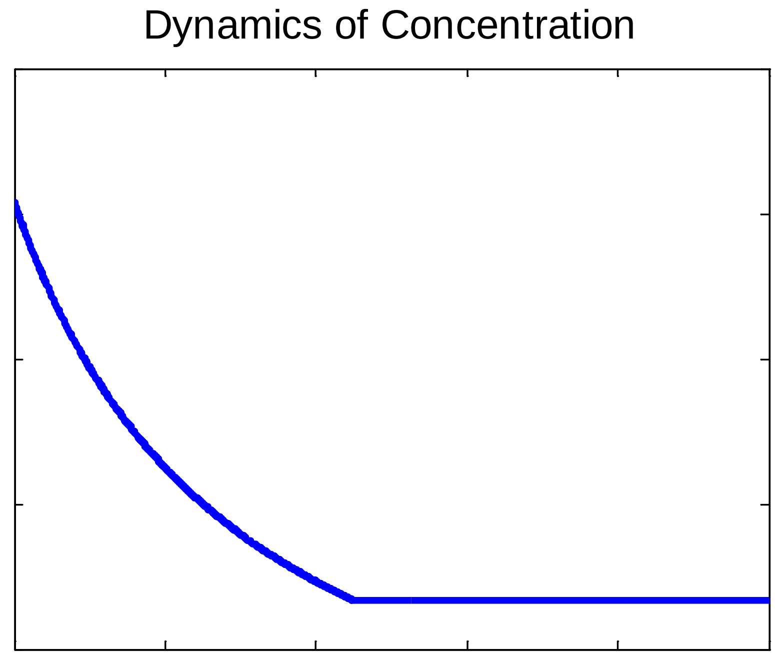
$$V \frac{dC_A}{dt} + C_A \frac{dV}{dt} = (C_{A1} F_1 + C_{A2} F_2) - C_{A3} F_3$$

$$\frac{dC_A}{dt} = \frac{(C_{A1} F_1 + C_{A2} F_2) - C_{A3} F_3 - \cancelto{0}{C_A \frac{dV}{dt}}}{V}$$

E3 – Mixer Results







E4 –CSTR Dynamics Results