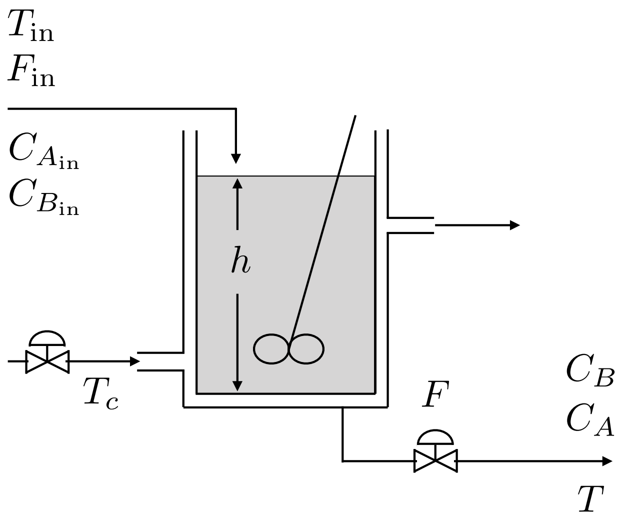
CHEM-E7225/2020-2021: Exercise 01

Task 1 (Explicit integration methods).
Consider a perfectly mixed continuous stirred tank chemical reactor (CSTR) in which an irreversible first-order reaction $A \to B$ occurs in liquid phase (see figure). The reactor's temperature T is regulated with an external cooling system. The controlled variables are the level h of the tank and the concentration of species A. The manipulated variables are the temperature T_c of the coolant and the outlet flowrate F. See G. Pannocchia and J.B. Rawlings. Disturbance models for offset-free MPC. *AIChE J.*, 49(2): 426–437, 2003.



Mass and energy balances lead to the following nonlinear dynamics

$$\frac{dC_A(t)}{dt} = \frac{F_{\text{in}}\left(C_{A_{\text{in}}} - C_A(t)\right)}{\pi r^2 h} - k_0 \exp\left(-\frac{E}{RT(t)}\right) C_A(t) \tag{1}$$

$$\frac{dT(t)}{dt} = \frac{F_{\text{in}}\left(T_{\text{in}} - T(t)\right)}{\pi r^2 h} + \frac{-\Delta H}{\rho C_p} k_0 \exp\left(-\frac{E}{RT(t)}\right) + \frac{2U}{r \rho C_p}\left(T_c(t) - T(t)\right) \tag{2}$$

$$\frac{dh(t)}{dt} = \frac{F_{\text{in}} - F(t)}{\pi r^2} \tag{3}$$

The state vector is $x(t) = (C_A(t), T(t), h(t))$ and the controls are $u(t) = (F(t), T_c(t))$. The disturbance vector $d(t) = (F_{\text{in}}, C_{A_{\text{in}}}, C_{B_{\text{in}}}, T_{\text{in}}) = (0.1, 1, 0, 350)$ is assumed constant in time and the components treated as known fixed parameters. The vector of model parameters in nominal operating conditions are the following

$$\theta_x = \begin{bmatrix} F_{\text{in}} \\ T_{\text{in}} \\ C_{A_{\text{in}}} \\ r \\ k_0 \\ E/R \\ U \\ \rho \\ C_p \\ \Delta H \end{bmatrix} = \begin{bmatrix} 0.1 & [\text{m}^3/\text{min}] \\ 350 & [\text{degK}] \\ 1 & [\text{kmol/m}^3] \\ 0.219 & [\text{m}] \\ 7.2 \times 10^{10} & [\text{min}^{-1}] \\ 8750 & [\text{degK}] \\ 54.94 & [\text{kJ / min} \cdot \text{m}^2 \cdot \text{K}] \\ 1000 & [\text{kg/m}^3] \\ 0.239 & [\text{kJ/kg} \cdot \text{K}] \\ -5 \times 10^4 & [\text{kJ/kmol}] \end{bmatrix}$$

We will adapt the starting code available in the archive `dynSim.zip` to compare different integration schemes.

- Adapt the main script and the functions to simulate the system above using all the schemes included in the main script. To verify the correctness of the implementation, plot the obtained trajectories of the system variables, when the system is subjected to varying control signals.
- Implement the RK4 scheme as a CasADi function and use it to perform the simulation. Again, verify the correctness of the implementation when the system is subjected to varying control signals.

Consider a simulation time of one hour (with 120 time-nodes, or more) and compare the accuracy of the solutions against what obtained using `ode15s`. A valid steady-state configuration to start the simulations is $x_{\text{ss}} = (0.878, 324.5, 0.659)$ and $u_{\text{ss}} = (0.1, 300)$.

Errata

- Error in the Arrhenius term of Eq. (2), the sign of the term inside parenthesis should be negative. The correct equation:

$$\frac{dT(t)}{dt} = \frac{F_{\text{in}}\left(T_{\text{in}} - T(t)\right)}{\pi r^2 h} + \frac{-\Delta H}{\rho C_p} k_0 \exp\left(-\frac{E}{RT(t)}\right) + \frac{2U}{r\rho C_p}\left(T_c(t) - T(t)\right);$$

- Error in the order of the valid steady-state conditions for the controls. The correct values

$$u_{\text{ss}} = (0.1, 300)\,.$$