Real Time Optimization & Model Predictive Control of CSTR

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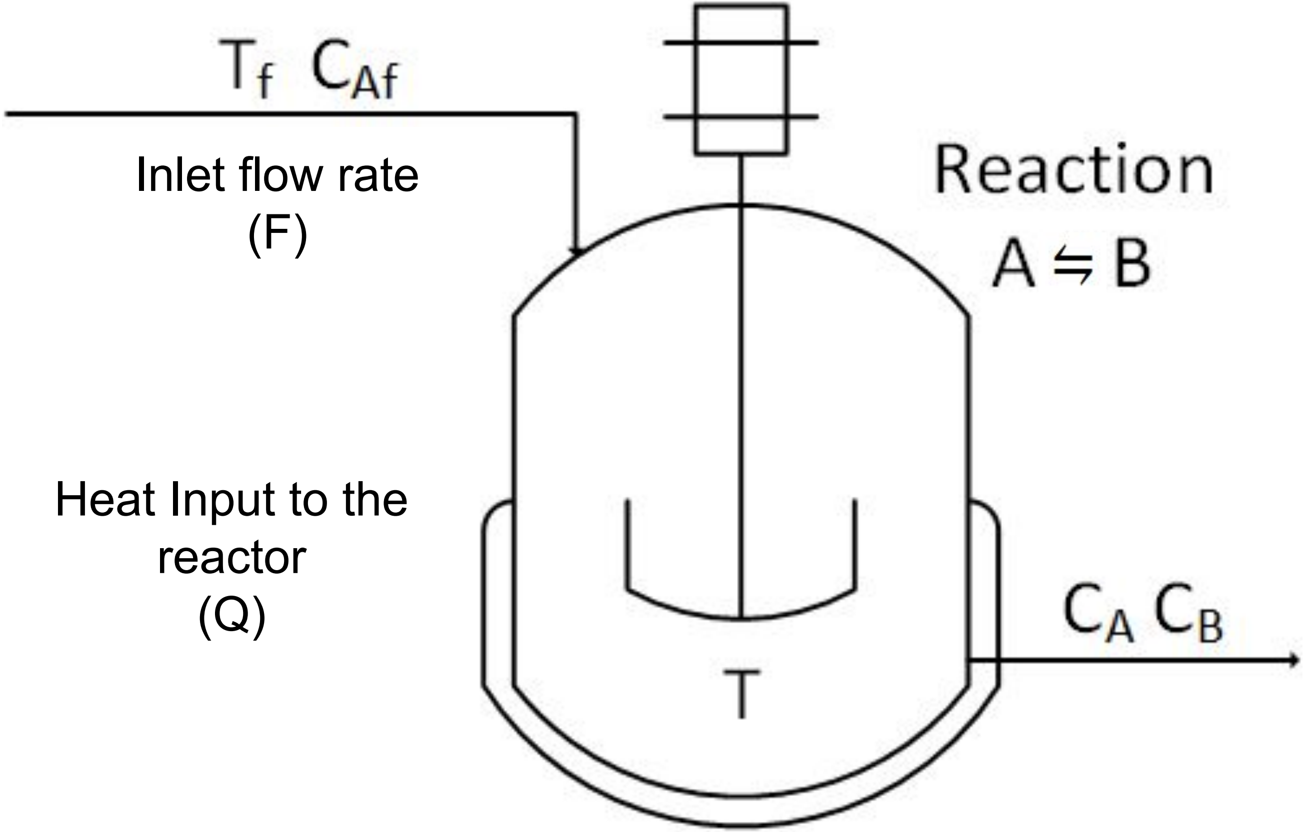
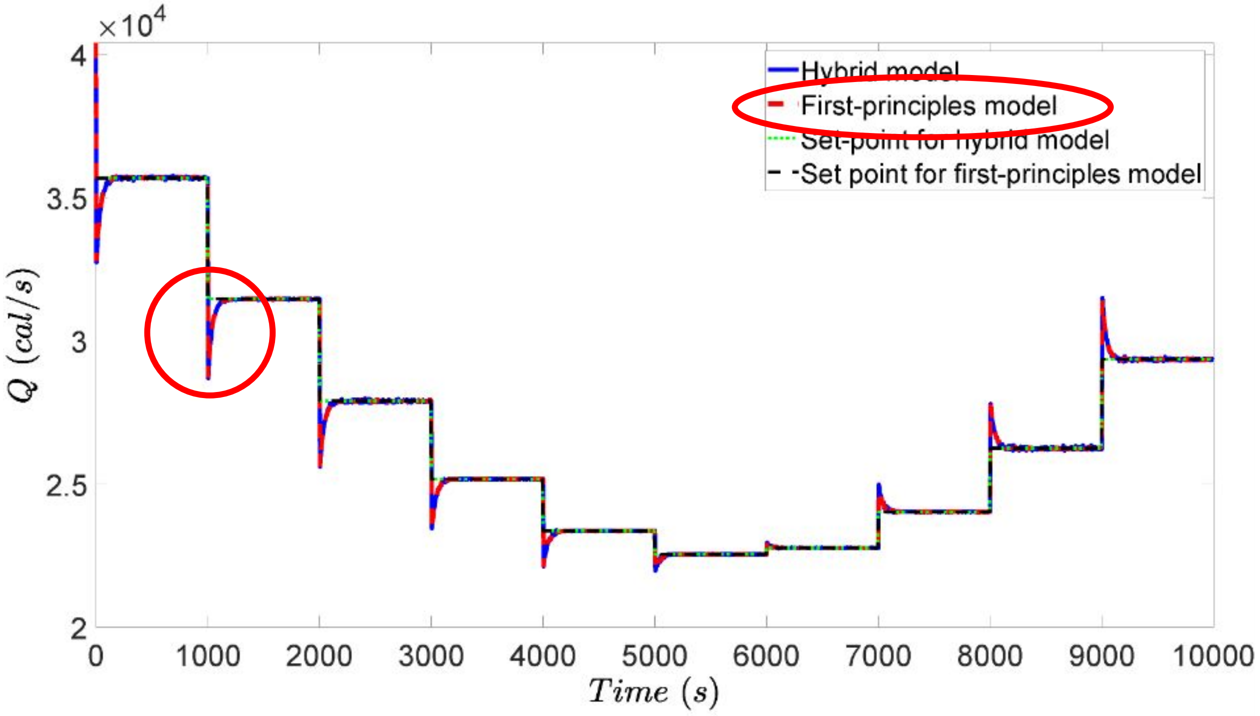
Objectives

- Modeling and simulation of ODE system
- Converting ODE model to discrete-time state-space representation
- Obtaining Step response model
- Develop the DMC algorithm
- Performing the ablation study
- Formulate the optimization problem for heat price variation
- Performing Real Time Optimization (RTO)
- Comparing Results

A CSTR with reversible reaction A⇋B is a nonlinear process with which we can implement MPC and RTO algorithms in order to minimize operating cost



Our study is a modification of a study done by Zhang et al that applied machine learning methods to RTO and MPC of nonlinear processes



RTO attempts to find a balance between reactant conversion and heat cost in order to calculate optimized setpoints

$$\min_{C_A,T,Q} \ Total\ cost = \frac{C_A}{C_{A_0}} + Heat\ Price \times Q$$

$$\text{s.t.} \quad 0 = \frac{1}{\tau}(C_{A_0} - C_A) - F_{NN}(C_A, C_B, T)$$

$$0 = -\frac{1}{\tau}C_B + F_{NN}(C_A, C_B, T)$$

$$0 = \frac{-\Delta H}{\rho C_P}F_{NN}(C_A, C_B, T) + \frac{1}{\tau}(T_0 - T) + \frac{Q}{\rho C_P V}$$

$$C_A \in [0, 1]$$

$$C_B \in [0, 1]$$

$$T \in [400, 500]$$

$$Q \in [0, 10^5]$$

Zhang et al showed that setpoints calculated with the neural network model were identical to ones calculated with the first principles model

ODE representation of our system

$$\frac{dC_A}{dt} = \frac{F}{V}(C_{Ao} - C_A) - k_A e^{\frac{-E_A}{RT}} C_A + k_B e^{\frac{-E_B}{RT}} C_B \qquad \text{Eqn. 1}$$

$$\frac{dT}{dt} = -\frac{\Delta H}{\rho C_P}\left(k_A e^{\frac{-E_A}{RT}} C_A - k_B e^{\frac{-E_B}{RT}} C_B\right) + \frac{F}{V}(T_0 - T) + \frac{Q}{\rho C_p V} \qquad \text{Eqn. 2}$$

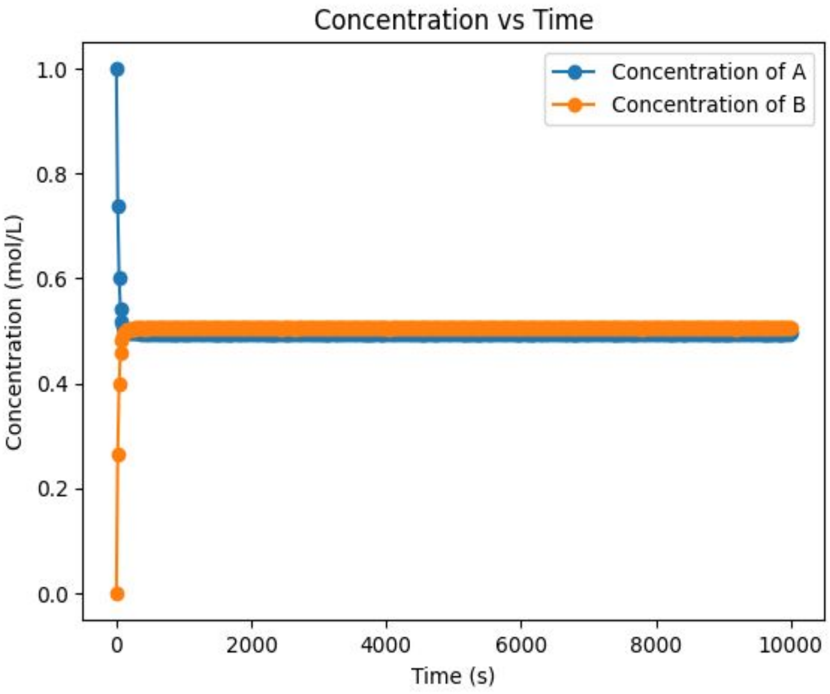
$$x = \begin{bmatrix} C_A - C_{As} \\ T - T_s \end{bmatrix} \qquad u = \begin{bmatrix} Q - Q_s \\ F - F_s \end{bmatrix} \qquad y = \begin{bmatrix} C_A - C_{As} \\ T - T_s \end{bmatrix}$$

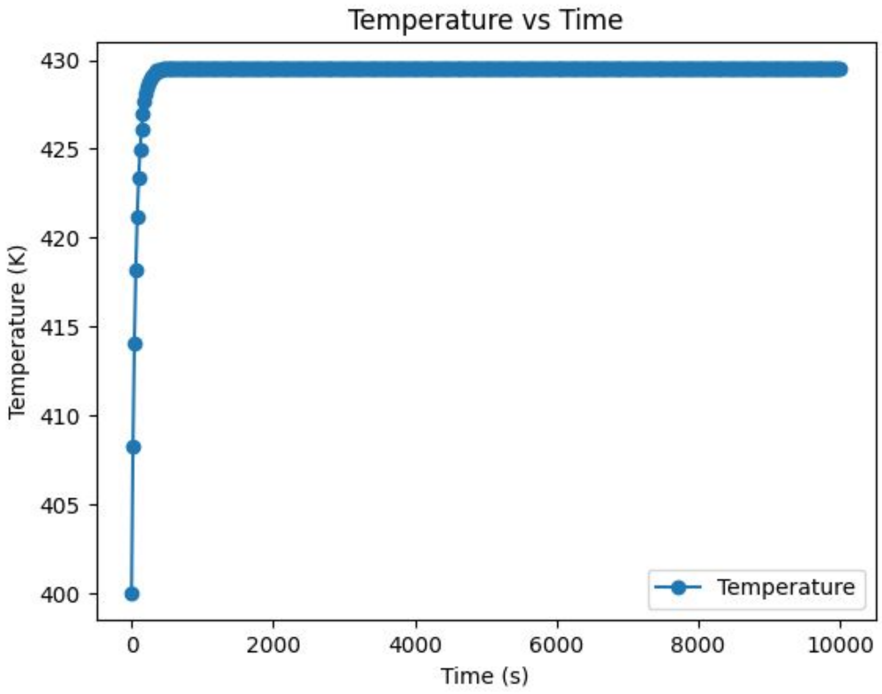
x are the States of the system

u are the inputs of the system

y are the outputs of the system

Steady state values were taken from Zhang et al and verified using solve.ivp





First, our system has to be depicted as a continuous state space model and converted to discrete time state space model

$$A_{11} = -\left(\frac{\Delta H}{\rho \times C_p}\right) * K_a * \exp\left(-\frac{E_a}{R * T_s}\right)$$

$$A_{12} = -\frac{F_s}{V} - K_a * \exp\left(\left(-\frac{E_a}{R * T_s}\right)\right)$$

$$A_{21} = -K_a * \exp\left(-\frac{E_a}{R * T_s}\right) * CA_s * \left(-\frac{E_a}{R * T_s^2}\right) + K_b * \exp\left(-\frac{E_a}{R * T_s}\right) * CB_s * \left(-\frac{E_a}{R * T_s^2}\right) * -\left(\frac{\Delta H}{\rho \times C_p}\right) + \frac{F_s}{V} * T_s$$

$$A_{22} = -K_a * \exp\left(-\frac{E_a}{R * T_s}\right) * CA_s * \left(-\frac{E_a}{R * T_s^2}\right) + K_b ** \exp\left(-\frac{E_a}{R * T_s}\right) * CB_s * \left(-\frac{E_a}{R * T_s^2}\right)$$

$$B_{11} = \frac{1}{\rho * C_p * V}$$

$$B_{12} = 0$$

$$B_{21} = \frac{T_0 - T_s}{V}$$

$$B_{22} = \frac{CA_0 - CA_s}{V}$$

$$C = \begin{bmatrix} C_{11} & C_{12} \\ C_{21} & C_{22} \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

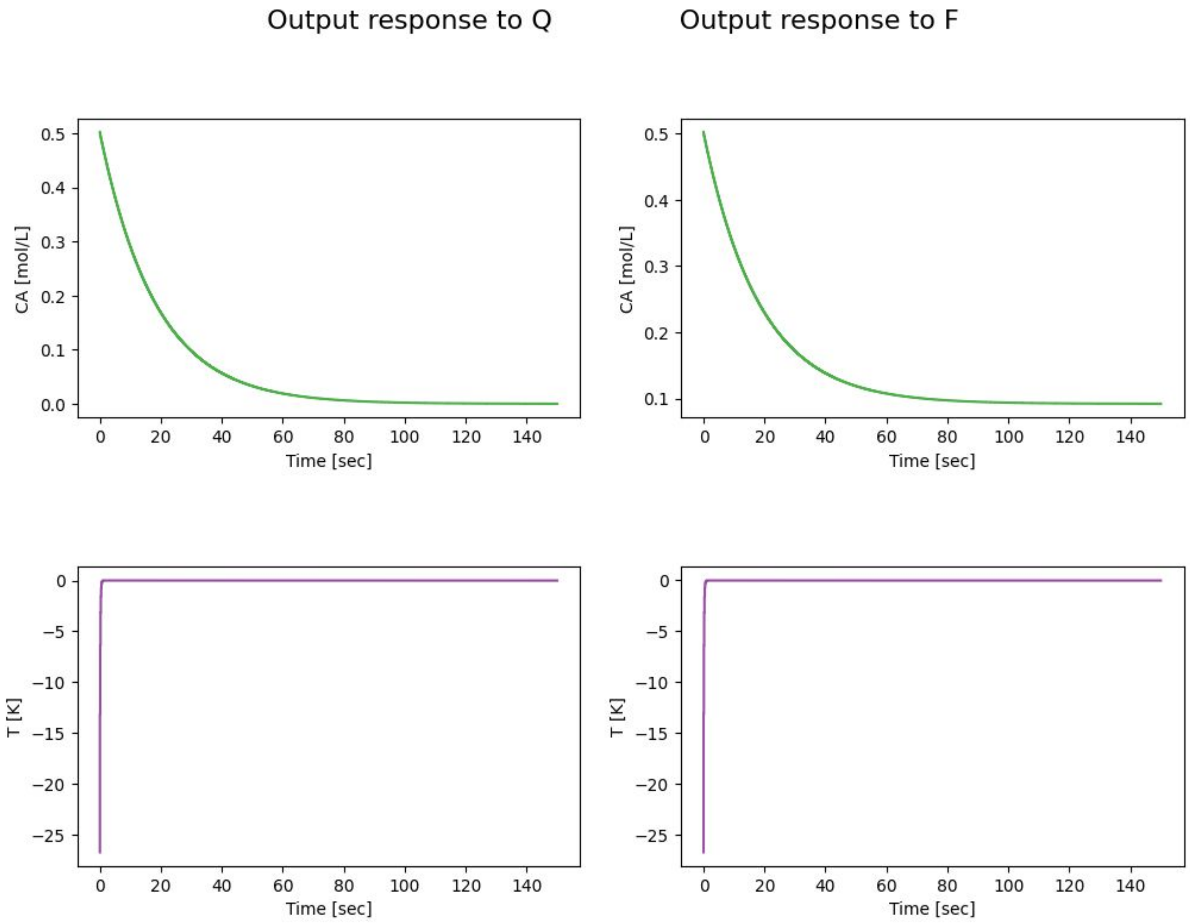
$$D = \begin{bmatrix} D_{11} & D_{12} \\ D_{21} & D_{22} \end{bmatrix} = \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix}$$

$$x(t) = Ax(t) + Bu(t)$$
$$y(t) = Cx(t) + Du(t)$$

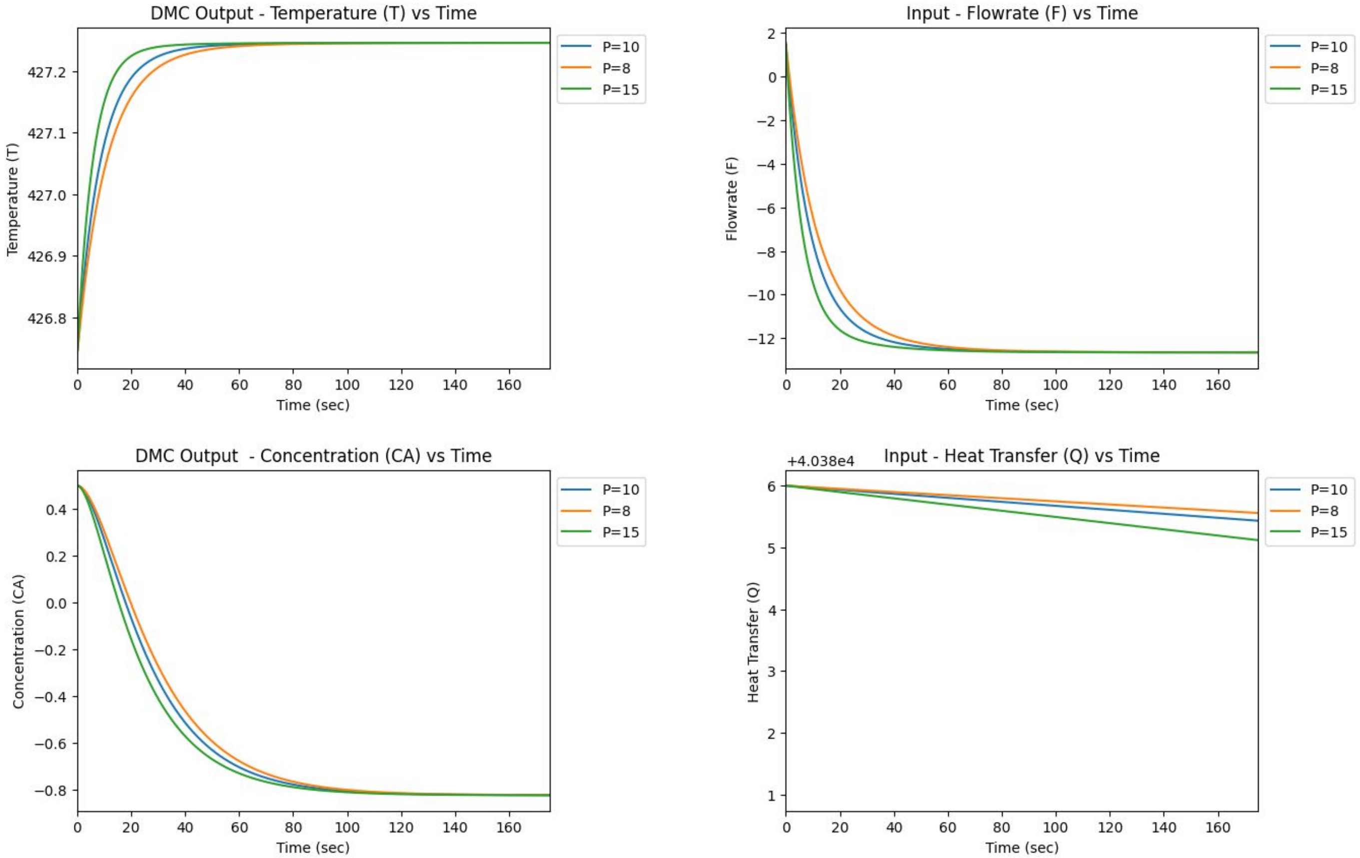
$$\longrightarrow$$

$$x(k+1) = \varphi x(k) + \Gamma u(k)$$
$$y(k) = Cx(k) + Du(k)$$

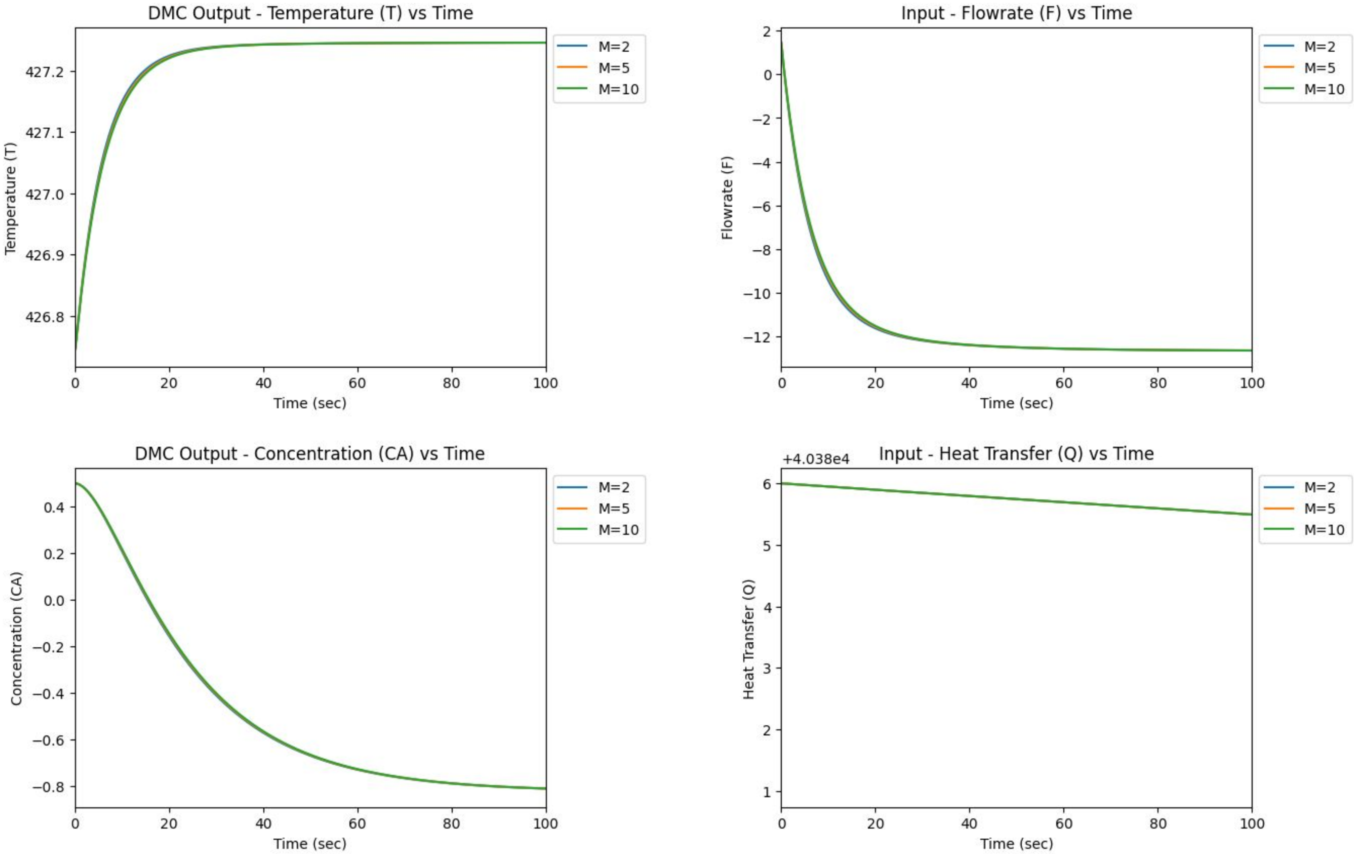
Step Response Model



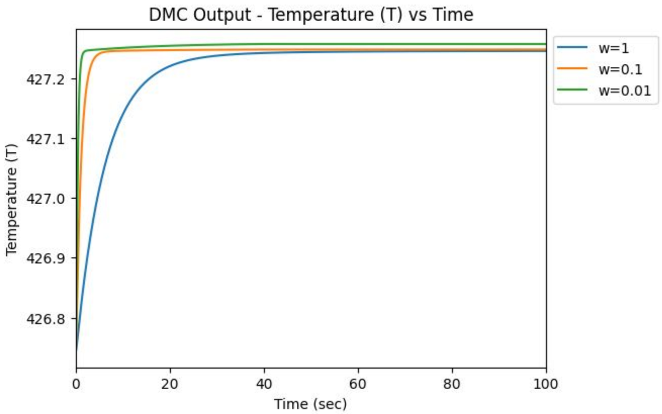
As the prediction horizon increases, the system reaches and settles at its new setpoint faster

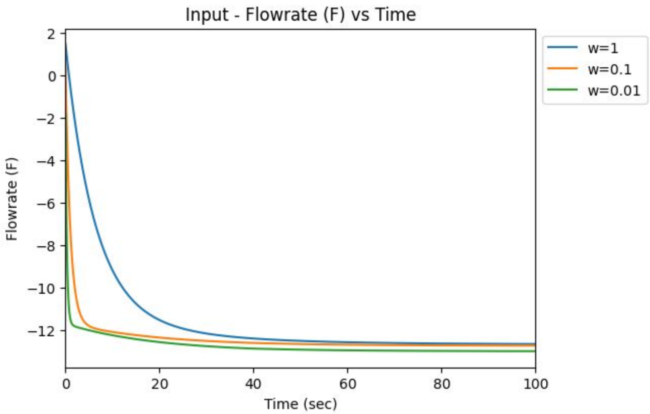


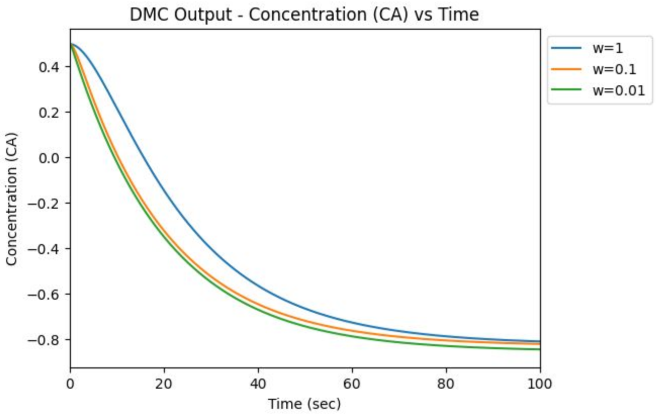
The control horizon has little effect on the performance of the system.

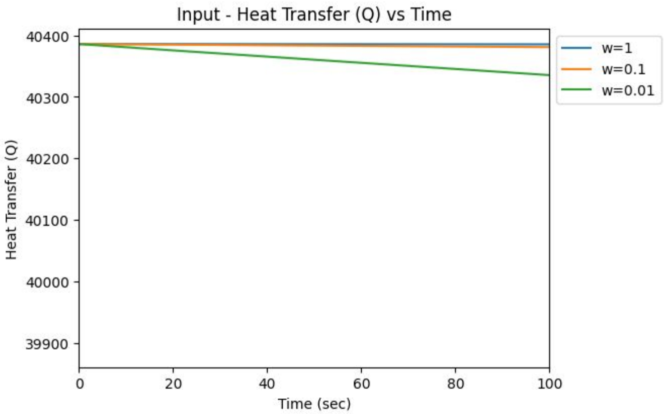


Lowering the weight leads to a faster settling time as well









RTO formulation for our CSTR system using ODE model

$$\min_{C_A,T,Q} \ Total\ cost = \frac{C_A}{C_{A_0}} + Heat\ Price \times Q$$

$$s.t.\ \ 0 = \frac{1}{\tau}(C_{A_0} - C_A) - k_A C_A e^{\frac{-E_A}{RT}} + k_B C_B e^{\frac{-E_B}{RT}}$$

$$0 = -\frac{1}{\tau}(C_B) + k_A C_A e^{\frac{-E_A}{RT}} - k_B C_B e^{\frac{-E_B}{RT}}$$

$$0 = \frac{-\Delta H}{\rho C_p}(k_A C_A e^{\frac{-E_A}{RT}} - k_B C_B e^{\frac{-E_B}{RT}}) + \frac{1}{\tau}(T_0 - T) + \frac{Q}{\rho C_p V}$$

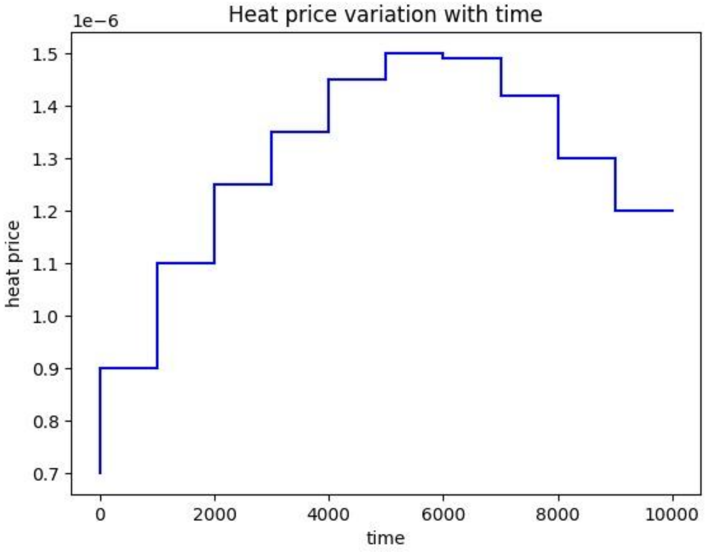
$$C_A \in [0, 1]$$

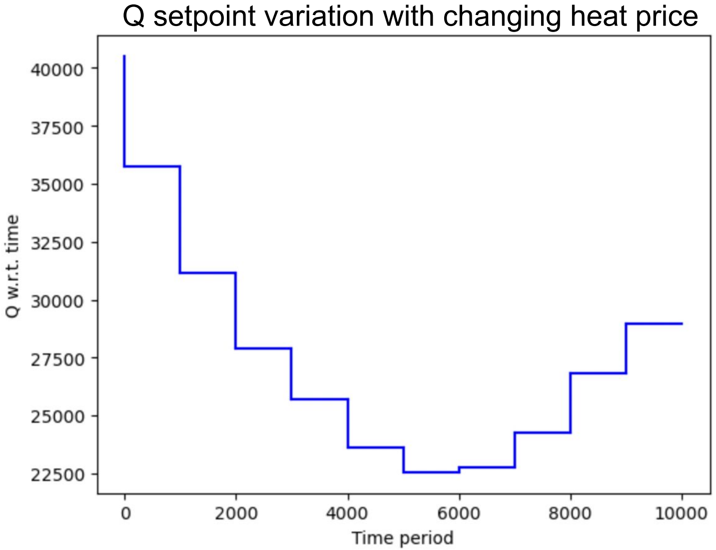
$$C_B \in [0, 1]$$

$$T \in [400, 500]$$

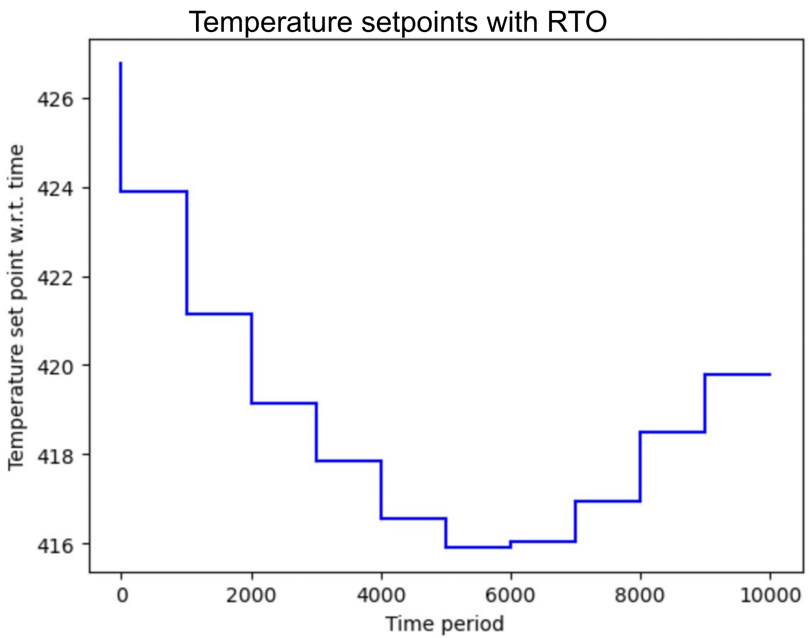
$$Q \in [0, 10^5]$$

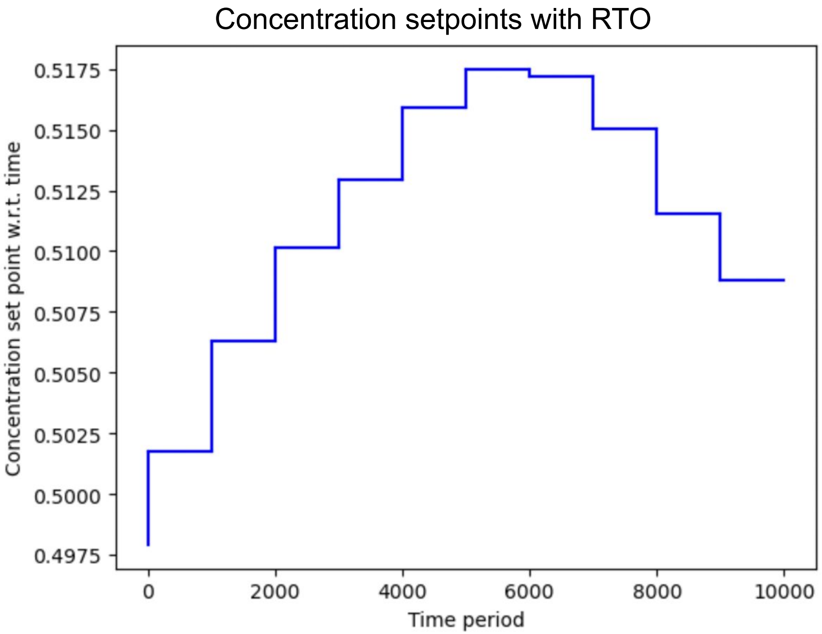
As the heat price increases initially, the optimization algorithm decreases the Q.





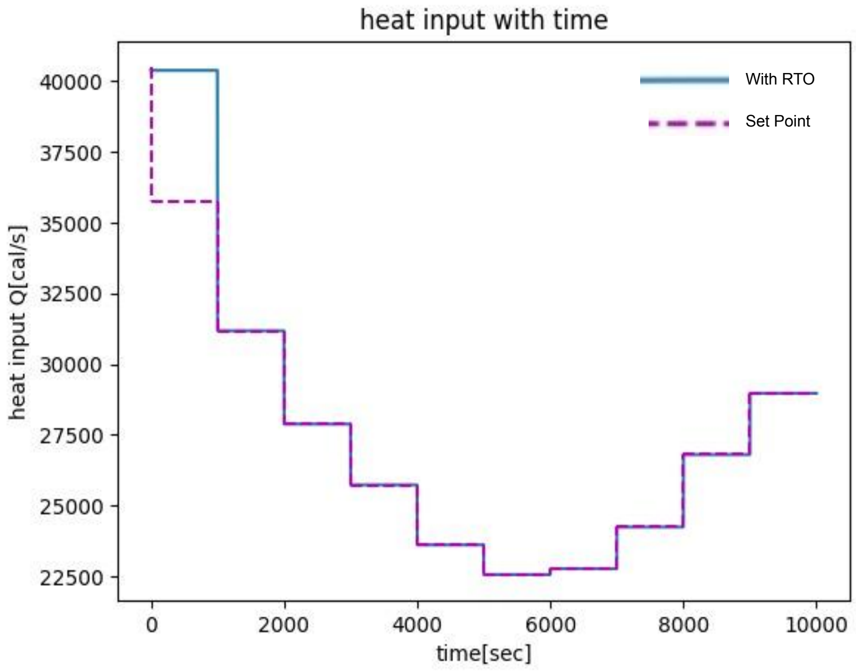
As heat price increases, RTO calculates lower setpoints for temperature and higher setpoints for concentration of A



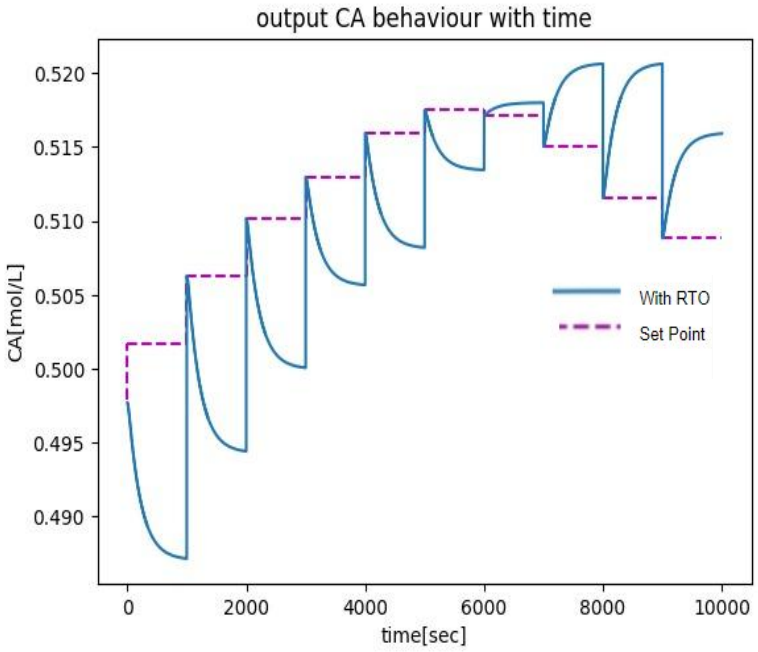


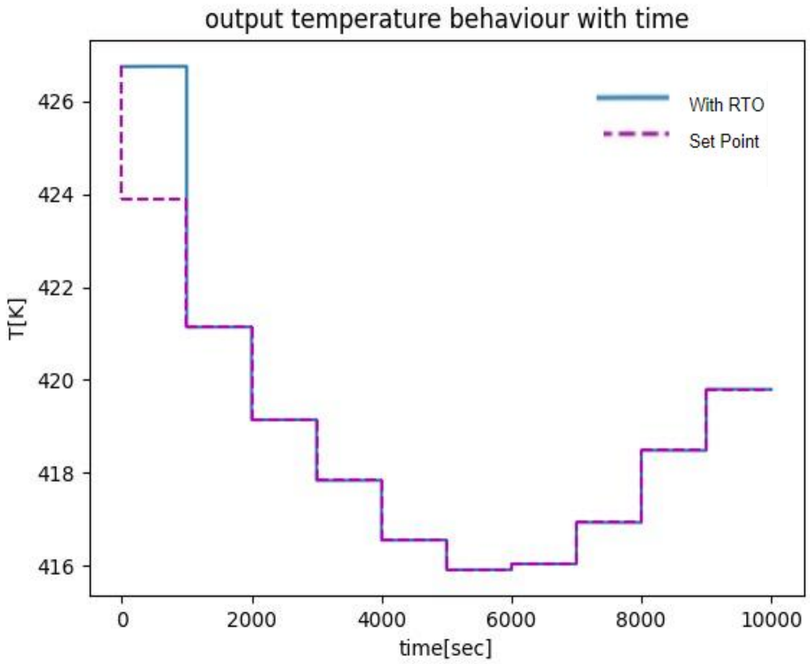
RTO integration with the DMC algorithm

Objective: To drive the system towards the optimal set points to keep the total cost low at all times.

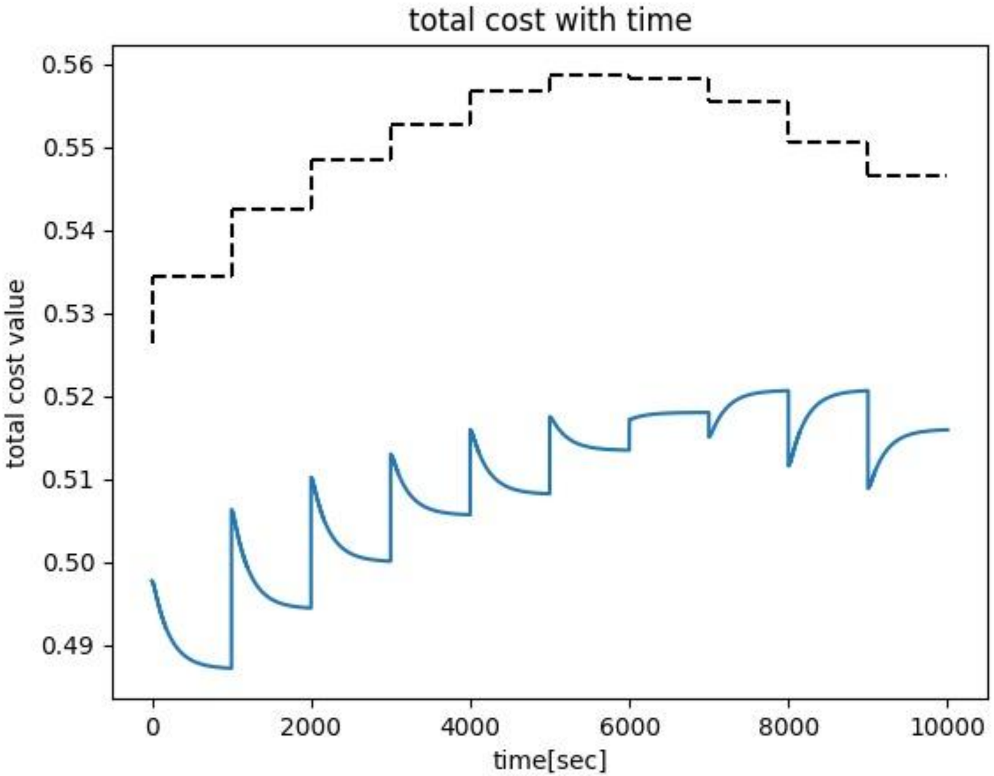


Upon implementing DMC over all time periods, we get the following real-time concentration and temperature plots





Cost comparison



Conclusions

- Significance of implementation of Real Time Optimization.
- Successful control of the output variables, while controlling the min cost, on fluctuating heat prices.
- Challenges due to difference in magnitude.
- Non-linearity might be one of the issues.
- Constraint optimization
- Future should include applying different MPC strategies to the system

References:

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