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Optimal online control of a semibatch reactor with varying prediction horizon

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Abstract

The model predictive control (MPC) is an advanced control technique that is able to perform linear control on multi-variable system subject to physical and operational constraints. For systems that can be adequately modelled by linear models, the MPC has become a widely used control technique and remain the de-facto standard advanced control technique in process industries.

However, industrial processes often do not display ideal behaviour and should rather be modelled as nonlinear in order to represent the system more accurately. A solution to this is to utilise the non-linear model predictive control (NMPC) that that is capable of addressing nonlinear behaviour. This controlling technique does however have several challenges associated with it, such as greater computational time than the MPC and difficulties calculating a global solution.

For this project an optimisation problem of a chemical reaction in a semibatch reactor producing a desired product C was simulated for an hour with the use of an NMPC and Plant model coded in the programming language of Julia. Integration of the states which the NMPC required was performed with orthogonal collocation utilising Gauss-Radau collocation points. Additionally, with a functional NMPC, a case study inspecting the effect of varying the length of the prediction horizon on the problem output was conducted.

Based off the plotted optimisation outputs, the results indicated that the coded NMPC was capable of solving the optimisation problem, as the constraints of the inputs,states, and algebraic values were not violated and the production of C stricly increased throughout the simulation. The results of the case study indicated that a prediction horizon of length $N = 15$ appeared to be the most cost-effective alternative that was able to predict future states of the semi-batch reactor with sufficient accuracy.

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Nomenclature

Acronyms

Table 1: List of Acronyms

	Description	Section
DAE	Differential Algebraic Equation	2.1
IPOPT	Interior Point Optimizer	2.2
JuMP	Julia for Mathematical Programming	2.2
MPC	Model Predictive Control	1.1
NMPC	Nonlinear Model Predictive Control	2.1
NLP	Nonlinear Programming	2.1
ODE	Ordinary Differential Equation	2.2
SS	Steady State	2.1

Units

Table 2: List of Units

Unit	Description	Section
g	Gram	3.1
h	Hour	3.1
J	Joule	3.1
k	Kilo	3.1
K	Kelvin	3.1
kW	Kilowatt	4.1
L	Litre	3.1
m	Meter	3.1
mol	Mol	3.1

Latin letters

Table 3: List of Latin letters

Symbol	Unit	Description	Section
A_W	m^2	Inner surface area covered with reaction mixture	3.1
Ca	[mol/L]	Concentration of A	3.1
Cb	[mol/L]	Concentration of B	3.1
Cb_{in}	[mol/L]	Input concentration of B	3.1
Cc	[mol/L]	Concentration of C	3.1
C_P	[kJ/gK]	Specific heat capacity of the reactor contents	3.1
$Cc0$	[mol/L]	Initial concentration of C	3.1
dt	[h]	Sampling instant	3.1
h	[-]	Scaling parameter (orthogonal collocation)	2.2
H	[kJ/mol]	Enthalpy	3.1
K	[L/molh]	Reaction constant	3.1
M	[-]	Weighting Matrix	2.2
N	[-]	Prediction horizon	3.2
$\dot{Q}_{\text{K}}$	[kJ/h]	Cooling input	3.1
r	[m]	Radius of cross-section of inner reactor	3.1
T_{in}	[K]	Temperature of inflow to reactor	3.1
T_J	[K]	Jacket Temperature	3.1
T_R	[K]	Reactor Temperature	3.1
V_R	[L]	Reactor volume	3.1
u_k	[-]	Manipulative variable at each sampling instant	3.2
$\dot{V}_{\text{in}}$	[L/h]	Inflow input	3.1
x_k	[-]	State trajectory at each sampling instant	3.2

Greek letters

Table 4: List of Greek letters

Symbol	Unit	Description	Section
α	[L/h]	heat-transfer coefficient between the reactor and jacket	3.1
$\Delta\dot{Q}_K$	[kJ/h]	Variable cooling input at each sampling instant	3.2
$\Delta\dot{V}_{\text{in}}$	[L/h]	Variable inflow input at each sampling instant	3.1
ϵ_k	[-]	Slack variable at each sampling instant	3.2
π	[-]	Pi, Mathematical constant	3.1
ρ	[g/L]	Density of reactor contents	3.1

1 Introduction

1.1 Motivation

In the industrial sector there is often a desire to maximize the profit of an eventual production line while at the same time minimizing the costs of running it. Another term of this is production optimisation and there are many factors that has to be considered in order to run the production site optimally in an economic sense. These factors can be classified within the categories of short or long term objectives of the operation. Some examples of the former can be adjusting the plant accordingly to randomly inflicted disturbances or running the plant optimally in real time. On the other hand examples of long-term objectives are planning which product to produce for the customer and how. Figure 1 illustrates the hierarchical decision system and the different layers associated with it that has to be addressed if optimal operation, at for instance, an industrial plant is to be realised (Darby et al. 2011).

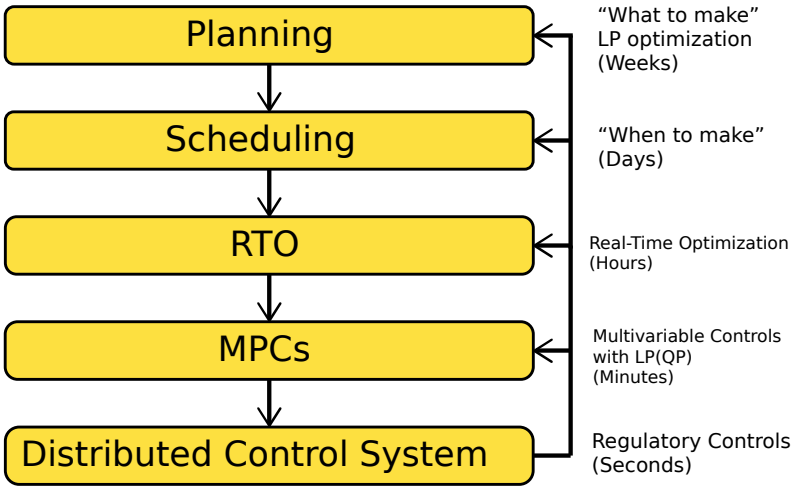


Figure 1: Source: Mark Darby, et al. "RTO: An overview and assessment of current practice." Journal of Process Control 21 (2011) 874–884.

For an industrial system there will always exist a degree of uncertainty as processes do not have ideal behaviour in the real world. Random external disturbances such as a change in the room temperature, humidity, or pressure can for instance affect a chemical reaction in a reactor. The process therefore require an advanced control method that is able to ensure optimal operation despite the uncertain external factors that the system is prone to. The control method also has to be able to operate optimally despite different constraints that limit the system operation. A widely used control technique in the industry is the model predictive control (MPC) which is able to fullfill the aforementioned requirements through predicting future states of the system and providing optimal inputs accordingly. However, the main drawback of this control technique is that it requires an accurate dynamic model of the system, something which can be considered an expensive practice.

Another issue that has to be addressed is how extensive the prediction of the MPC should be. On one hand the shorter the prediction horizon is, the less computational effort the NMPC will require. The opposite will be the case for a longer horizon and the accuracy and performance trade-off has to be considered when designing an MPC.

1.2 Goals of the project

The main goal of the project is to define a functioning NMPC that ensures optimal operation of an industrial application. After that has been completed, the next goal of the project is to conduct a case study by varying the prediction horizon in order to investigate the effect the length of it has on the NMPC performance and accuracy. Apart from these objectives, a more academic goal of the project is to familiarise the student with the NMPC-concept and implementation of it. This is to be done in order to prepare the student for an eventual master thesis that can build upon this project by conducting research on more unexplored topics within the field of system control and optimisation.

2 Theory

2.1 Nonlinear model predictive control

A natural choice of control technique to investigate for this project is the previously mentioned model predictive control (MPC). The control technique is already widely used in the industry for process optimisation, so it make sense that the project work is performed with a technique that is applicable to the real world. The main appeal of a MPC is its ability to effectively control large multi-variable processes that are limited by physical and operational constraints. Additionally the method is considered to be robust, meaning that the MPC is still able to perform optimal control if an external disturbance was to be applied. (Johansen 2011*a*)

Unlike for instance Steady-State control, the MPC do not have to achieve steady state after a disturbance occurs before it is able to perform optimal control. This saves time, making the MPC a more economic choice than SS-control methods. On the other hand, implementation of the dynamic model of the former requires greater effort than the latter, so there is an accuracy and performance trade-off that has to be considered as well.

A MPC utilises linear dynamic models, and the accuracy of these can be questionable, as industrial processes often do not inherit ideal behaviour that can be approximated to linear models. A more representative solution for this project would be to utilise a Nonlinear Model Predictive Controller (NMPC) that is able to control nonlinear dynamic models. On the other hand Nonlinear Programming (NLP) require greater computational effort and it is not guaranteed that they are able to calculate a feasible solution. The solvers for these type of problems are often dependent on the provided initial condition in order to achieve convergence towards a specific solution. (Johansen 2011*b*)

The overall operational objectives of a MPC are: (Seborg et al. 2011)

1. Prevent violations of input and output constraints
2. Drive some output variables to their optimal set points, while maintaining other outputs within specified ranges
3. Prevent excessive movement of the input variables
4. Control as many process variables as possible when a sensor or actuator is not available,

and Figure 2 illustrates the operational goals of an NMPC:

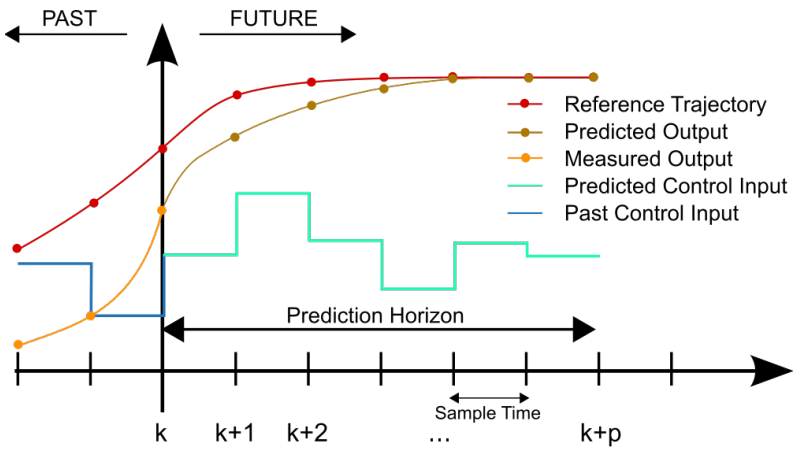


Figure 2: Overview of the NMPC operation

First the objective function, its corresponding constraints and the operational goal are defined for the NMPC. The plant then provides the dynamic model that consists of a series of ordinary differential equations (ODEs) and eventual algebraic equations (DAEs) to the NMPC. Before the NMPC can calculate the optimal input sequence u it must obtain information about the current state of the system. To achieve this, the given dynamic model from the plant is integrated, something that can be performed by various methods. For now it is worth mentioning that orthogonal collocation is used for this project and this choice of method is further elaborated in Section 2.2.

With the integrated states the NMPC calculates the input sequence u that minimises the negative cost function. This sequence has a specific length and the NMPC will only provide the first element of it to the plant. Calculating a long sequence, but only implement the first element may seem inefficient, but the philosophy behind this is that the NMPC should continuously know the actions it is to perform in the future. This ensures operational predictability while maximising the cost function, a trait that is deemed beneficial.

Figure 3 illustrates the optimal solution sequence u that is calculated and continuously updated at every sampling instant of the prediction horizon:

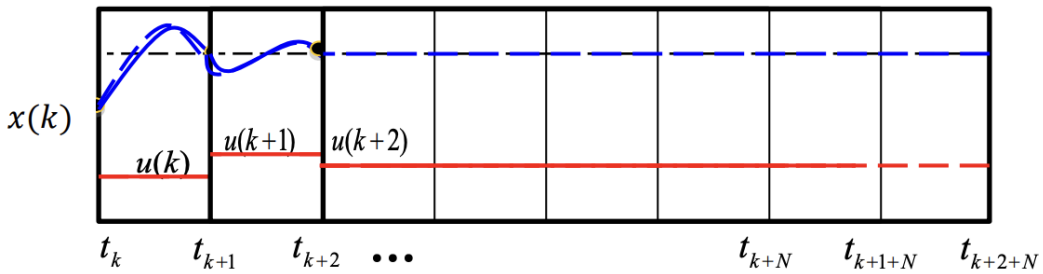


Figure 3: Illustration of the state trajectory x and input sequence u at every sampling instant k over the prediction horizon. The NMPC only provides the first element of the input sequence to the Plant

The length of this horizon determines how far in the future the NMPC is able to predict the states. With a functional NMPC, it is this length variable that later is to be varied in the case study. The eventual results of this will indicate the effect the length has on NMPC performance and accuracy

Finally, Figure 4 provides a visual summary of the aforementioned components that is required to be defined in order to solve the optimisation problem.

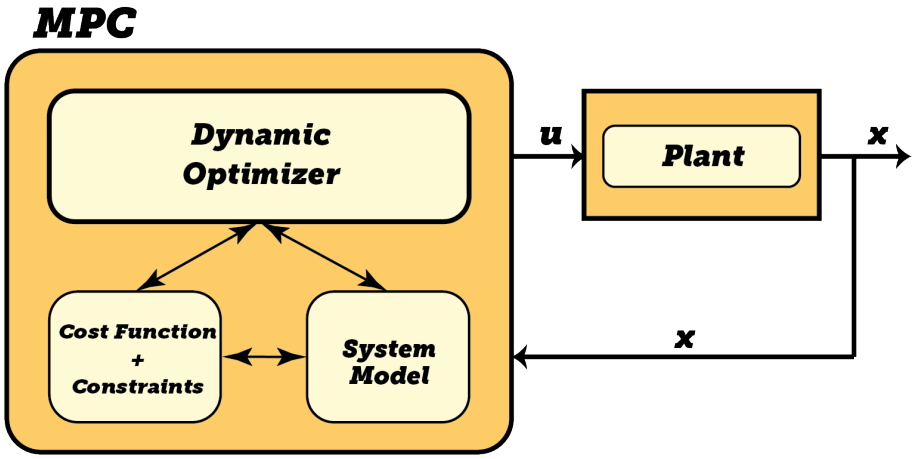


Figure 4: The different components that an NMPC requires for optimal control. The MPC receives a set of ODEs from the Plant before integrating them and calculating an optimal sequence u. The first element is provided to the Plant which then calculate measurable values of the states, x, using an ODEsolver.

2.2 State integration with orthogonal collocation

The operational goal of a NMPC is to maximise a given cost function and calculate optimal inputs for the control system that results in a robust,economic, and reliable operation of the process. If the NMPC is to calculate and provide optimal inputs, it requires information about the current states of the system.

With a provided plant model consisting of a series of ODEs and DAEs, the NMPC integrates the system and acquire the required information about the states. With this, an optimal input sequence u, that maximises the operational goal of the NMPC is then calculated. In the case of this project, the optimize! function from the JuMP package in Julia is utilised in order to achieve this.

The input sequence is then provided to the Plant function which with this information calculates measurable values of the states. This is done with an ODEsolver, or more specifically the solve-function from the "DifferentialEquations" package in Julia. Additionally, the ODEsolver is provided initial condition of the states and time step dt arguments from the NMPC.

The output state trajectory x from the Plant is then stored in global vectors and plotted in order to visually illustrate the system behaviour over time. This can for instance be useful for digital control softwares surveying a production process for instance. Finally the plant provides an updated plant model to the NMPC again, thereby closing the loop. Figure 5 provides a visual overview of the plant and an overview of the interaction between it and the NMPC.

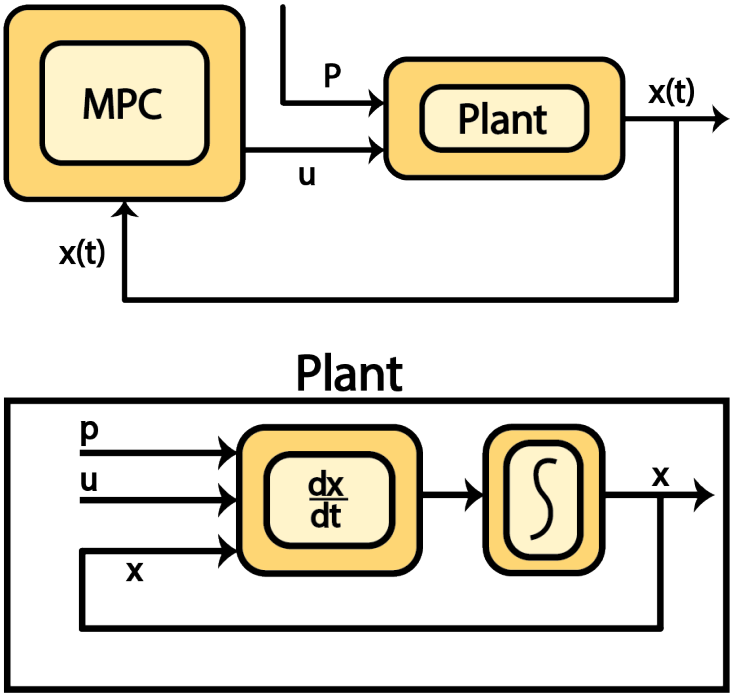
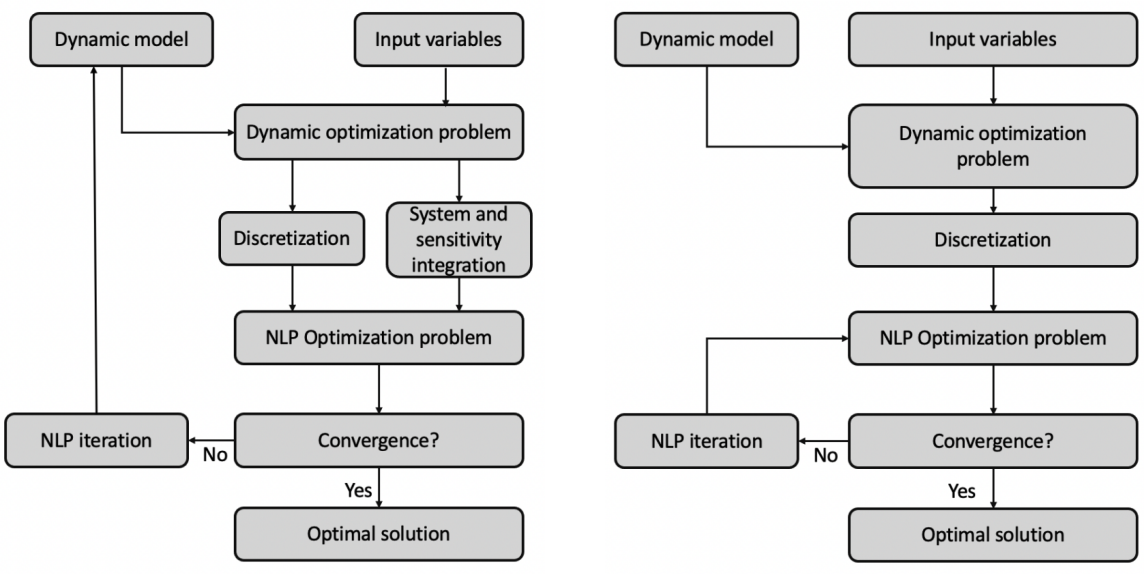


Figure 5: Overview of the plant and the interraction between it and the MPC

There are various methods for the NMPC to calculate the optimal control u, such as single shooting, multiple shooting and orthogonal collocation. Each of these method have their respective advantages and disadvantages and the preferred choice is often the one that is the most computationally effective for the problem and yield a sufficient accuracy. For instance multiple shooting proves to be effective for optimisation problems that require a large amount of iterations and consists of a few number of variables. On the other hand the opposite is the case for orthogonal collocation which is preferred when the NLP-problem is large and fewer iterations are required (Tysland 2020).

Multiple shooting and orthogonal collocation are widely used methods in the industry and there are disagreements about which one is superior when calculating the state trajectory for the NMPC. The main difference is how the method integrate the system of ODEs that it is provided. Multiple shooting utilises an embedded integrator to integrate the states while orthogonal collocation uses the optimiser to perform the integration by evaluating the ODEs at specific collocation points. Agnes Tysland compared these two methods in her article Tysland (2020) and Figure 6 provides an illustration of the difference.



Multiple shooting

Orthogonal collocation

Figure 6: Source: Tysland, Agnes, et. al. "A Comparison of Multiple Shooting and Collocation Approaches using Nonlinear Model Predictive Control"

As illustrated in Figure 6, the main difference is that multiple shooting utilises an embedded integrator to calculate the states unlike orthogonal collocation which uses the optimiser to perform the same task. For this project orthogonal collocation is used to integrate the states because of its low computational cost and accuracy. The main idea of orthogonal collocation is to divide the prediction horizon into finite elements, which again are further divided based off the number of collocation points that is to be used. For this project the Gauss-Radau collocation points, $t = [01151, 0.6449, 1.0000]$, are utilised as they remove the need to interpolate at the end of every finite element since the last collocation point is 1.0.

The set of differential Equations from the Plant that is to be integrated is:

$$M \begin{bmatrix} \dot{x}_1 \\ \dot{x}_2 \\ \dot{x}_3 \end{bmatrix} = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} - \begin{bmatrix} x_0 \\ x_0 \\ x_0 \end{bmatrix}, \tag{1}$$

where M is the weighting matrix. The state trajectory can be approximated as a polynomial with Equation 1

$$x(t) \approx A + Bt + \frac{1}{2}Ct^2 + \frac{1}{3}Dt^3, \tag{2}$$

and the derivative $\dot{x}$ can be calculated simply by differentiating with the respect to t:

$$\dot{x}(t) \approx B + Ct + Dt^2. \tag{3}$$

An example of an approximation state trajectory, x, is illustrated in Figure 7.

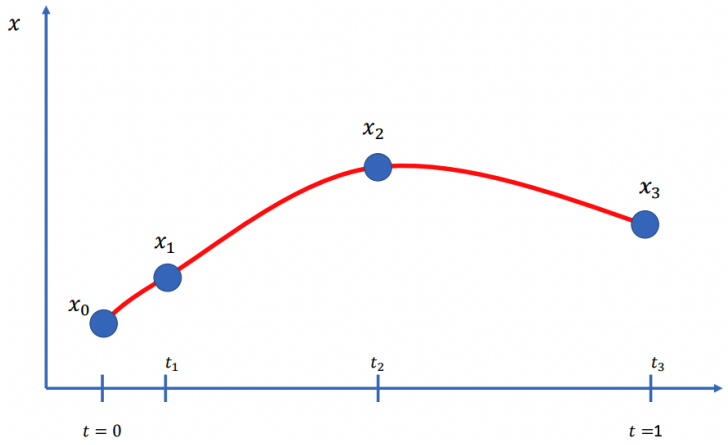


Figure 7: An example of a polynomial approximated by orthogonal collocation

The goal is then to solve the aforementioned equations with respect to x. To do this the weighting matrix M first has to be calculated. Inserting Equation 2 and 3 into Equation 1 yields

$$M \begin{bmatrix} B + Ct_1 + Dt_1{}^2 \\ B + Ct_2 + Dt_2{}^2 \\ B + Ct_3 + Dt_3{}^2 \end{bmatrix} = \begin{bmatrix} A + Bt_1 + \frac{1}{2}Ct_1{}^2 + \frac{1}{3}Dt_1{}^3 \\ A + Bt_2 + \frac{1}{2}Ct_2{}^2 + \frac{1}{3}Dt_2{}^3 \\ A + Bt_3 + \frac{1}{2}Ct_3{}^2 + \frac{1}{3}Dt_3{}^3 \end{bmatrix} - \begin{bmatrix} x_0 \\ x_0 \\ x_0 \end{bmatrix} \tag{4}$$

If B,C, and D is factorised and the A is set equal to the initial condition, $A = x_0$, Equation 7 can be simplified to:

$$M \begin{bmatrix} 1 + t_1 + t_1{}^2 \\ 2 + t_2 + t_2{}^2 \\ 3 + t_3 + t_3{}^2 \end{bmatrix} \begin{bmatrix} B \\ C \\ D \end{bmatrix} = \begin{bmatrix} t_1 + \frac{1}{2}t_1{}^2 + \frac{1}{3}t_1{}^3 \\ t_2 + \frac{1}{2}t_2{}^2 + \frac{1}{3}t_2{}^3 \\ t_3 + \frac{1}{2}t_3{}^2 + \frac{1}{3}t_3{}^3 \end{bmatrix} \begin{bmatrix} B \\ C \\ D \end{bmatrix} \tag{5}$$

The weighting matrix M can then be calculated to be equal to:

$$M = \begin{bmatrix} t_1 + \frac{1}{2}{t_1}^2 + \frac{1}{3}{t_1}^3 \\ t_2 + \frac{1}{2}{t_2}^2 + \frac{1}{3}{t_2}^3 \\ t_3 + \frac{1}{2}{t_3}^2 + \frac{1}{3}{t_3}^3 \end{bmatrix} \begin{bmatrix} 1 + t_1 + {t_1}^2 \\ 2 + t_2 + {t_2}^2 \\ 3 + t_3 + {t_3}^2 \end{bmatrix}^{-1} \tag{6}$$

The weighting matrix is therefore calculated based on the position of the utilised collocation points. Finally, the state trajectory x can be approximated with M from Equation 6 inserted in to Equation 1.

$$\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} x_0 \\ x_0 \\ x_0 \end{bmatrix} + hM \begin{bmatrix} f(x1, u1, z1, p1) \\ f(x2, u2, z2, p2) \\ f(x3, u3, z3, p3) \end{bmatrix}, \tag{7}$$

where x represents the states, u the inputs, z the algebraic variables, and p the parameters of the process that is to be optimised. h is a scaling parameter that is utilised if the collocation points range is not between 0 and 1. This is however the case for Gauss-Radau collocation points and this parameter is therefore set to be $h = 1$. With orthogonal collocation, the maximisation of the cost function becomes a nonlinear optimisation problem. To solve this an IPOPT solver from the JuMP package in Julia is utilised (Ågotnes 2019).

3 Implementation and case study

3.1 The dynamic model

In general, calculating the solution of the NLP can be considered computationally expensive since it has to compute a large number of variables at every iteration in a horizon (Rolf Findeisen 2002). Because of that, the nonlinear optimisation problem that is to be investigated in this project should have a dynamic model that consists of a small number of variables. Additionally the problem should be conceptually simple so that an undergraduate student is able to solve it. An optimisation problem based off a semibatch reactor with an already existing dynamic model derived by (Thangavel et al. 2020) fulfils these criteria and is therefore to be the basis for this project.

The chemical reaction that takes place in the semibatch reactor is

$$A + B \rightarrow C, \tag{8}$$

and an illustration of the semibatch reactor along with its state variables and inputs are given in Figure 8

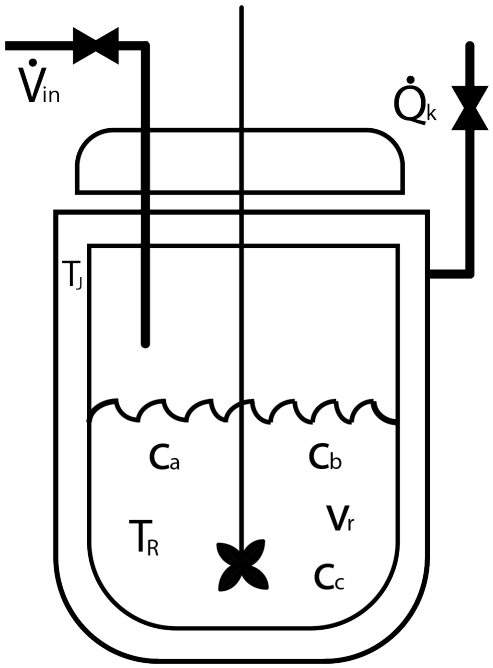


Figure 8: Illustration of the semibatch reactor and its jacket that is to be investigated for this project

As described in the article, the control task is to maximize the production of C along the prediction horizon while satisfying a series of constraints over a specific time period which in this case is 1.0 hour. The nonlinear model is derived from the mass balance of the reactor, molar balances of reactants A, and B, and energy balances of the reactor and the jacket. The differential equations of the states in the semibatch reactor are:

$$\dot{V}_{\mathrm{R}} = \dot{V}_{\mathrm{in}} \tag{9a}$$

$$\dot{c}_{\mathrm{A}} = -\frac{\dot{V}_{\mathrm{in}}}{V_R} c_A - K c_A c_B \tag{9b}$$

$$\dot{c}_{\mathrm{B}} = \frac{\dot{V}_{\mathrm{in}}}{V_R}(c_{\mathrm{B,in}} - c_B) \tag{9c}$$

$$\dot{T}_R = \frac{\dot{V}_{\mathrm{in}}}{V_R}(T_{\mathrm{in}} - T_R) - \frac{\alpha A_W (T_{\mathrm{R}} - T_J)}{\rho V_{\mathrm{R}} c_p} - \frac{K c_A c_B H}{\rho c_p} \tag{9d}$$

$$\dot{T}_J = \frac{\dot{Q}_K + \alpha A_W (T_R - T_J)}{\rho V_J c_p} \tag{9e}$$

while the algebraic equations are:

$$c_C = \frac{c_{A,0} V_{R,0} + c_{C,0} V_{R,0} - c_A V_R}{V_R} \tag{10a}$$

$$A_W = \pi r^2 + \frac{0.002 V_R}{r} \tag{10b}$$

where V_R denotes the volume of the reactor, and c_A,c_B and c_C represents the concentration of the components A,B and C respectively. T_R and T_J are the corresponding temperatures of the content inside the reactor and the heating jacket. A_W denotes the inner surface area of the reactor that is covered with the reaction mixture. This specific variable is weighted with 0.002 for unit conversion of L to m^3. Finally the manipulate variables, or control inputs, of the process are the inflow of reactants $\dot{V}_{\mathrm{in}}$ and the cooling power $\dot{Q}_k$ of the jacket. The rest of the variables are considered constant and are given in Table 1

Table 1: Plant Model parameters

Parameter	**Description**	**Value**	**Unit**
α	heat-transfer coefficient	1700	$\mathrm{kJK^{-1}h^{-1}m^{-2}}$
r	cross-section radius of inner reactor	0.092	m
ρ	density of the reactor contents	1000	$\mathrm{gL^{-1}}$
c_P	heat capacity of reactor contents	$4.2 \cdot 10^{-3}$	$\mathrm{kJg^{-1}K^{-1}}$
$c_{\mathrm{B,in}}$	input concentration of reactant B	3	$\mathrm{molL^{-1}}$
V_J	content volume in cooling jacket	2.22	L
T_{in}	temperature of inflow	300	K
$c_{C,0}$	initial concentration of the product C	0	$\mathrm{molL^{-1}}$

Additionally there are two parameters, the respective reaction enthalpy and constant, H and K, that occurs in Equation9b and 9d. It is described in the article that the value of these are not known precisely. This makes sense as different factors such as temperature and utilised catalysts have a significant impact on the kinetics of the chemical reaction(Key 2014). These parameters therefore represent an uncertainty and has to be estimated if the optimisation problem is to be solved. However, parameter estimation of uncertainties remain outside the scope of this project and the parameters have therefore been assumed to remain constant at the fixed values:

$$\mathbf{p}_0 = \begin{pmatrix} H \\ K \end{pmatrix} = \begin{pmatrix} -355 \frac{\text{kJ}}{\text{mol}} \\ 1.205 \frac{\text{l}}{\text{mol h}} \end{pmatrix} \tag{11}$$

According to the article the semibatch reactor is to run for an hour with a sampling instant of $dt = 0.05$, or every 3 minutes. The length of the prediction horizon for the initial optimisation problem is chosen to be $N = 20$ and because of the finite simulation time the optimisation problem has a shrinking horizon attribute. Finally, the required initial conditions of the states and algebraic variables are given in Table 1 and 2 while the initial inputs u_0 are assumed to be equal to 0.

3.2 Constraints and cost function

For the optimisation problem there are several physical constraints that has to be considered when maximising product C. For instance, the semibatch reactor has to have an upper bound on V_R in order to avoid spillover as the reactants are added with the inflow input V_{in}. There are also operational constraints as the control inputs V_{in} and Q_{K} have limited capability of adding inflow to the system and cooling the reactor jacket. A summary of the constraints of the system are given in Table 2 and Table 3:

Table 2: Upper and lower bounds of the states along with proposed initial conditions

State	Intial Condition	Lower Bound	Upper Bound	Unit
V_R	3.5	0	8	L
c_A	2	0	5	mol L^{-1}
c_B	0	0	5	mol L^{-1}
T_R	325	273	350	K
T_J	325	273	350	K

Table 3: Upper and lower bounds of control inputs

Control	Lower Bound	Upper Bound	Unit
$\dot{V}_{\text{in}}$	0	32.4	L h^{-1}
$\dot{Q}_{\text{K}}$	-9000	0	kJ h^{-1}

Additionally it is given that the temperature of the reactor, T_R has to remain in the temperature range $322K \leq T_R \leq 326K$. Finally the volume of the reactor, V_R must not exceed 7L in order to avoid spillover. As mentioned earlier, the goal of the NMPC is to minimise the negative cost of the production of C along the prediction horizon. The cost function that is to minimised for the semibatch reactor optimisation problem is:

$$\underset{\mathbf{x}_k, \mathbf{u}_k, \epsilon_k}{min} \sum_{k=1}^{N} -c_C V_R + 0.0154(\Delta \dot{V}_{in,k})^2 + 5.5 \times 10^{-5}(\Delta \dot{Q}_k)^2 + 10^6 {\epsilon_{k,[1]}}^2 + 10^{10} {\epsilon_{k,[2]}}^2 \quad (12)$$

where $\Delta \dot{V}_{\text{in,k}} = \dot{V}_{\text{in,k}} - \dot{V}_{\text{in,k-1}}$ and $\Delta \dot{Q}_k = \dot{Q}_k - \dot{Q}_{k-1}$. These terms denotes the regularisation terms. As nonlinear programming tend to have a multitude of local solutions (Balaman 2019), the control inputs has to be penalised in order to force the optimiser to converge towards a specific local solution. Without the regularisation terms the optimiser will continuously evaluate all of the local solutions in the feasible set, something that can be considered counterproductive when trying to achieve numerical convergence towards an unique solution. The regularisation terms also ensure that the control input profile remain smooth as they penalise the cost function the greater the difference between subsequent control inputs are.

Additionally, slack variables are introduced in the cost function as ϵ_1 and ϵ_2. Their purpose is to provide flexibility to the optimiser in the border region of constraint violation. For instance, complications could arise for the optimiser if it was to be close to violating the volume constraint. The slack variables can therefore be added or subtracted to the states in order to avoid constraint violation should it be necessary. However, operating close to constraint violation is considered unfavourable and the usage of the slack variables are therefore heavily penalised with their respective weights.

In summary the cost function given in Equation 12 is to be subject to the following constraints:

$$x_{k+1} = f(x, u_k, d_k) \tag{13a}$$
$$322 \leq T_{R,k} + \epsilon_{k,[1]} \leq 326 \tag{13b}$$
$$V_{R,k} + \epsilon_{k,[2]} \leq 7 \tag{13c}$$
$$-1 \leq \epsilon_{k,[1]} \leq 1 \tag{13d}$$
$$-0.01 \leq \epsilon_{k,[2]} \leq 0.01 \tag{13e}$$
$$\underline{u} \leq u_k \leq \overline{u} \tag{13f}$$
$$x_s = {x_s}^m \tag{13g}$$
$$\tag{13h}$$

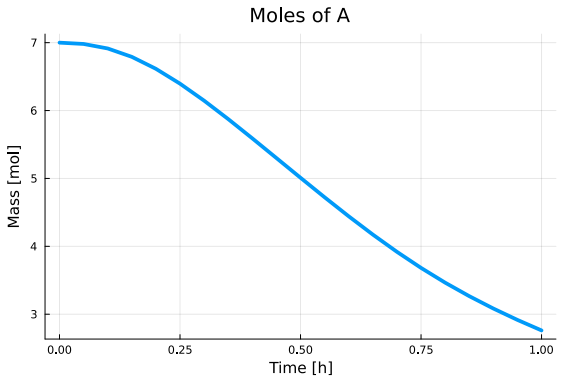
3.3 Case study with varying prediction horizon

After the NMPC has been initialised and the output verified, the next goal of the project is to investigate the effect the length of the prediction horizon has on the NMPC performance and accuracy. For the previous optimisation problem, the length of the prediction horizon is fixed at $N = 20$. However, for the case study, the optimisation problem is to be solved 3 additional times with $N = 5$, $N = 10$ and $N = 15$. The resulting states, inputs, and algebraic values are then to be plotted accordingly in order to visually interpret the output.

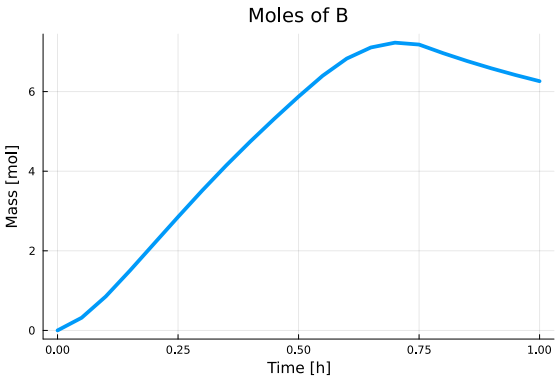
4 Results and Discussion

4.1 Output from the optimisation problem

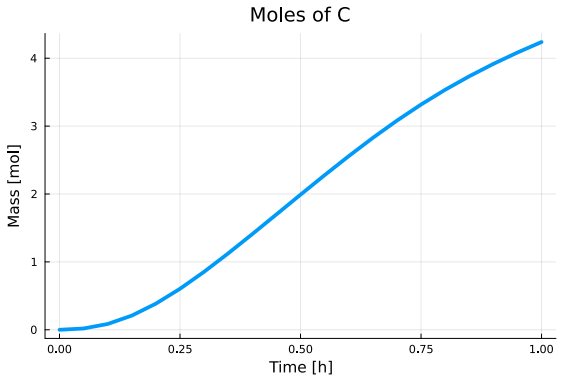
With the optimisation settings described at the end of Section 3.1, the NMPC was able to calculate a local optimal solution at each sampling instant. The resulting trajectories of the states, inputs, and algebraic variables are given in Figure 9. The trajectory of A_W was not plotted as the algebraic value is only linearly dependent on V_R, which resulted in an almost identical control profile that was only shifted along the y-axis.



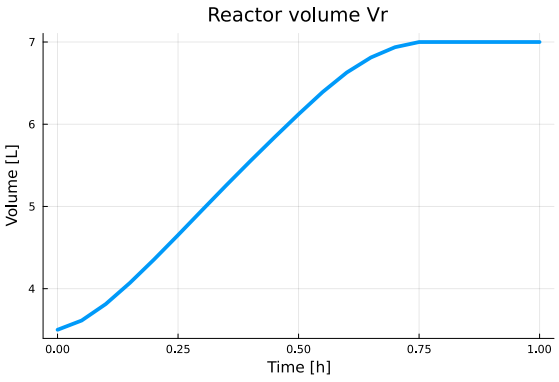
(a) Trajectory of moles of A



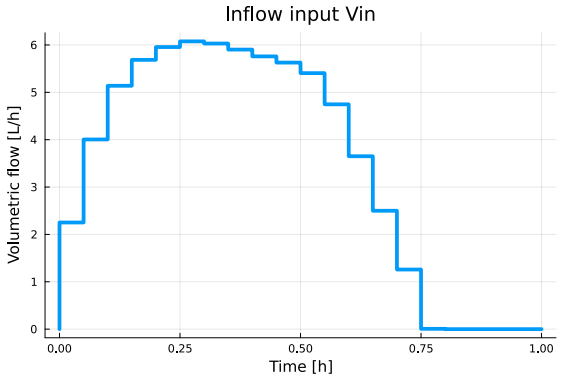
(b) Trajectory of moles of B



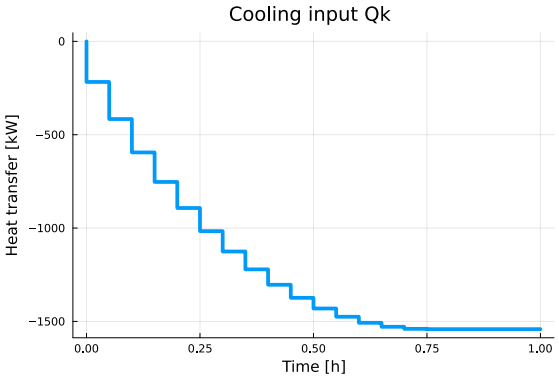
(c) Trajectory of moles of C



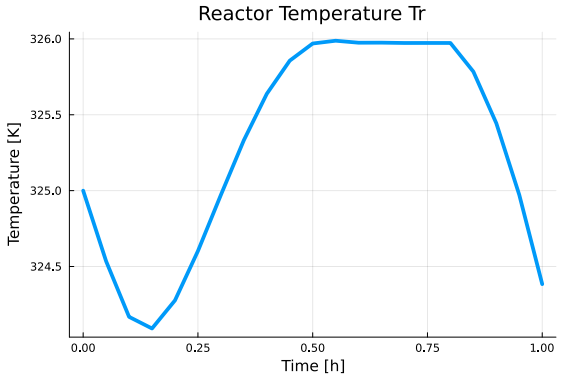
(d) Trajectory of reactor volume V_R



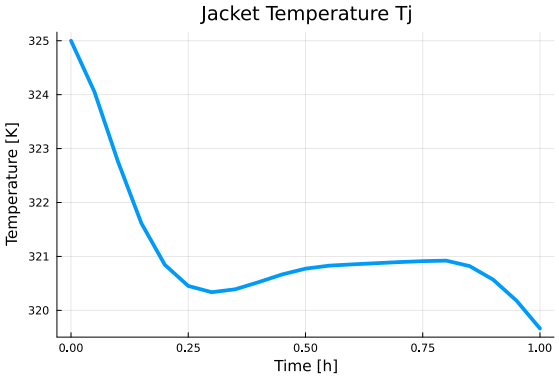
(e) Trajectory of the inflow input V_{in}



(f) Trajectory of the cooling input Q_{k}



(g) Trajectory of reactor temperature T_R



(h) Trajectory of jacket temperature T_J

Figure 9: Trajectory of the optimisation problem. The V_R and T_R constraints are not violated and the production of C also remains strictly increasing over prediction horizon.

Based off the figures, it is apparent that the NMPC provides outputs that appear physically reasonable. It is also observed that the optimisation do not violate the constraints given in Equation 13. For instance the reactor volume V_R do not exceed 7L at any point during the simulation and the reactor temperature T_R remains within the small range of 322-326K.

As the reactor only contains A at the beginning of the simulation, it makes sense that amount of A consistently decrease over time as it it consumed in the chemical reaction. In the beginning there is no B in the reactor and the moles of it increases over time as it is added with the inflow input. At the end of the horizon, around at the same time that the reactor volume constraint becomes active, the moles of B achieves its maxima before it decreases. This is most likely because of the shrinking horizon attribute of the optimisation that makes the NMPC produce C more aggressively towards the end of the horizon. At this point the consumption rate of B becomes greater than the inflow of it, something which results in the moles of B starting to decrease.

According to Figure 9d, the V_R constraint becomes active at the end of the simulation at $t \approx 0.75$. This is caused by the increasing aggressiveness of the NMPC as it tries to maximise the production of C by adding more reactants with the inflow input. The length of the horizon and the effects it has on the optimisation is explained more thoroughly in Section 4.2. Regardless of the varying degree of aggressiveness throughout the simulation, the NMPC achieves its operational goal, something that Figure 9c confirms considering that the number of moles of C strictly increases over the shrinking horizon.

The control inputs appear to display expected behaviour and both remain well within their respective bounds. The inflow input steadily increases before it starts to decline after approximately $t \approx 0.25$. This is most likely because the NMPC tries to maximise C through the inflow input in the beginning, only for it to later predict that this behaviour will eventually end up violating the volume constraint. The cooling input Q_{K} seem to consistently decrease before it settles at a constant value around -1550kW at the end of the horizon. This is because of the regularisation term $\Delta\dot{Q}_K$ in the cost function that penalises the cooling input over the prediction horizon.

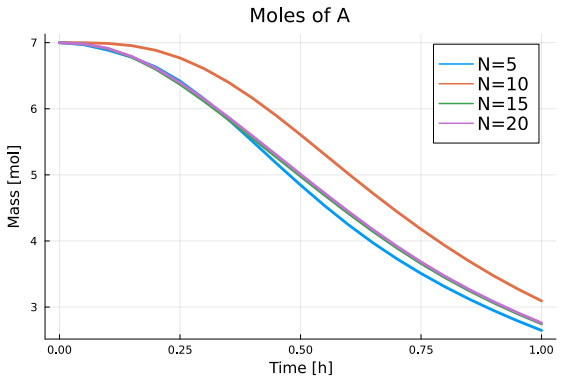
It may be worth noting that both T_R and T_J reach their respective local minima at approximately $t \approx 0.25 \pm 5$. The temperature of the inflow is lower than the temperature of the mixture since the chemical reaction has a negative enthalpy and transfer heat to the system. In the beginning of the simulation, the concentration of reactant B is low, which results in less generated heat from the chemical reaction and lower T_R values. As the concentration of B increases with the inflow input, generated heat in the reactor increases which results in higher T_R values. At $t \approx 0.50$ it is observed that the reactor temperature T_R constraint almost becomes active for a period of about 15 minutes. Finally, at around $t \approx 0.75$, the volume constraint becomes active, which means that the inflow input,

and thereby the addition of reactants, terminates. With this decrease of reactants, the generated heat from the chemical reaction decreases and T_R as well.

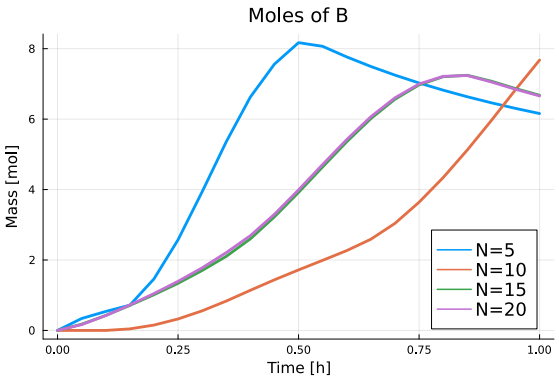
The jacket temperature T_J appear to have a similar trajectory to T_R, most likely caused by heat transfer between the jacket and reactor. In the beginning of the horizon T_J decreases significantly as the cooling input Q_{K} is applied on the system. At $t \approx 25$, the generated heat from the reaction increases, to the point where the cooling input Q_{K} is not able to fully counter the temperature increase of the reactor. As a result of this, the jacket temperature T_J increases in accordance with T_R until the latter begins to decrease again at the end of the horizon.

4.2 Outfrom from case study

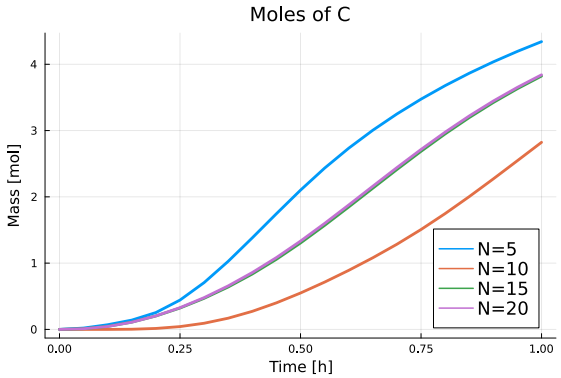
As described in Section 3.3, a case study investigating the effect of the length of the prediction horizon had on the optimisation problem output was conducted. Simulations with different predictions horizons $N = 5$, $N = 10$, $N = 15$ and $N = 20$ were ran and the results are given in Figure 10



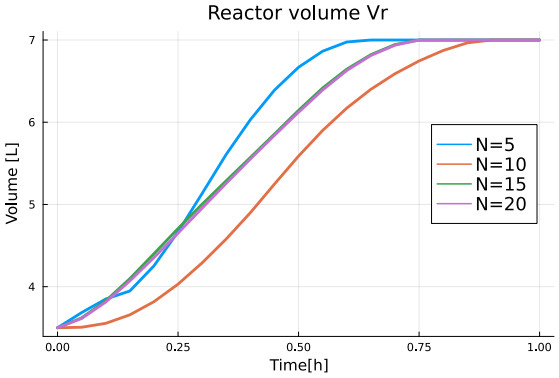
(a) Moles of A with varying lengths of prediction horizon



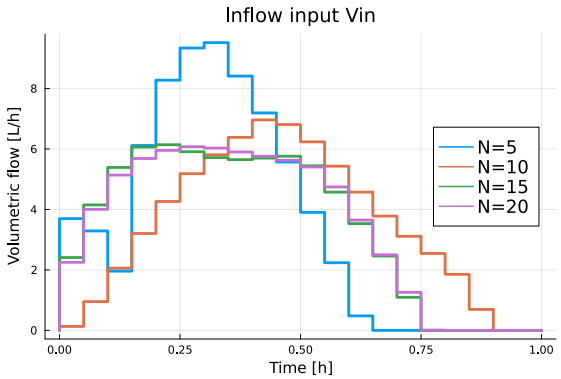
(b) Moles of B with varying lengths of prediction horizon



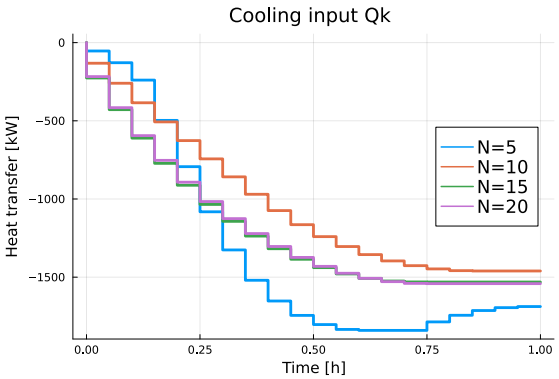
(c) Moles of C with varying lengths of prediction horizon



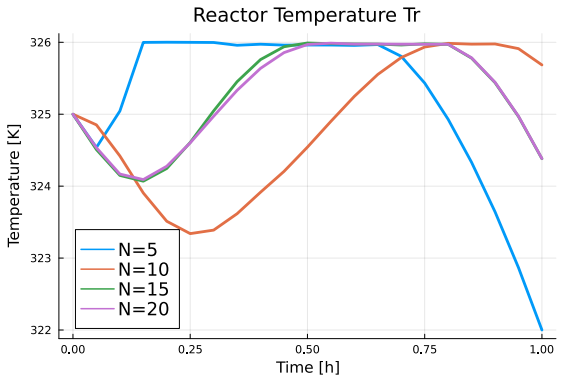
(d) Reactor volume V_R with varying lengths of prediction horizon



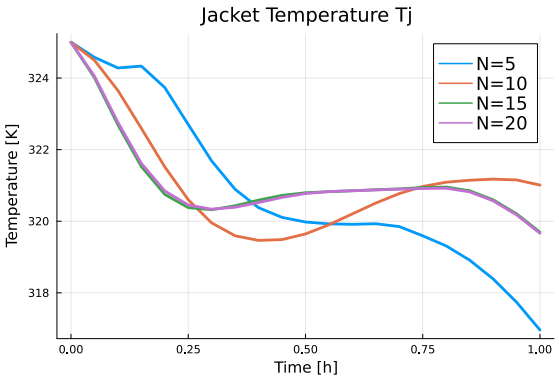
(e) Inflow input V_{in} with varying lengths of prediction horizon



(f) Cooling input Q_{K} with varying lengths of prediction horizon



(g) Reactor temperature T_R with varying lengths of prediction horizon



(h) Jacket temperature T_J with varying lengths of prediction horizon

Figure 10: Output of the states,inputs, and algebraic variables with varying prediction horizons

Compared to the output discussed in Section 4.1, most of the states,inputs and algebraic variables follow the same trajectory from the case base with $N = 20$, albeit with varying accuracy. Based off Figure 10, it appears that the length of the control horizon has a significant effect on the trajectory of the states, inputs and algebraic variables. One of the more interesting results are that the shortest prediction horizon with $N = 5$ yields the most C. The control profiles of V_{in} and Q_{K} are interesting as well as the prediction length appear to have a significant effect on how aggressive the control inputs of the NMPC are. A quantification of the input usage and production of C is summmarized in Table 4

Table 4: Quantification of the input usage and produced C for each case. The former was obtained by summarising the absolute value of each control input over the prediction horizon

Case	**Produced C [mol]**	**Sum of $\dot{V}_{\text{in}}$ inputs [L]**	**Sum of $\dot{Q}_{\text{K}}$ inputs [kW]**
$N = 5$	4.342	70.000	26820.919
$N = 10$	2.823	70.000	20729.860
$N = 15$	3.822	69.999	24204.8239
$N = 20$	3.841	69.999	24102.6821

In summary, the main observations from these results is that the short horizon $N = 5$ yield the most aggressive control profiles, $N = 10$ appear to result in a over-conservative control profile with an insufficient response time, and finally $N = 15$ and $N = 20$ results in almost identical behaviour.

With a short prediction horizon of $N = 5$, the NMPC is not able to fully comprehend the long-term consequences of the actions it performs. For instance, in the beginning of the simulation the NMPC will immediately increase the inflow aggressively, as it believes it has to maximise C as quickly as possible for the short period of time it perceives. Because of this, the NMPC is not able to have a "long-term" control plan, which in turn may result in greater overshooting and excessive input usage. This is observed in Figure 10e and 10f where the control profile with $N = 5$ deviates significantly compared to the rest of the trajectories. As mentioned earlier, $N = 5$ yield the most C, but this aggressive behaviour may be infeasible for a long term operation, which is the case for the semibatch reactor.

On the other hand $N = 10$ appear to be much more conservative, almost to the point where it leads to sub-optimal operation with an insufficient response time. Additionally the prediction horizon length also yield significantly less C compared to $N = 5$,$N = 15$ and $N = 20$. A possible explanation for this is that the NMPC predict the future states more conservatively. However it is apparent that horizon with $N = 10$ remain insufficiently short, as it showcases sub-optimal behaviour with significantly longer response time compared to the other trajectories. The combination of conservative behaviour and a horizon that remain too short results in $N = 10$ being the least optimal choice.

The trajectories of $N = 15$ and $N = 20$ appear to represent a compromise between aggressive and conservative control. It also seem like the trajectories of $N = 15$ and $N = 20$ are almost identical which indicate that the length increase from the former to the latter do not yield any significant benefit performance-wise, but only extra computational effort. The increase from $N = 10$ to $N = 15$ appear to be improve the response-time, and thereby the overall performance of the NMPC. This, along with the non-unique output of $N = 20$ indicate that a prediction horizon with $N = 15$ is long enough to predict the future accurately and places the NMPC in somewhat of a sweetspot in the aggressive and conservative control trade-off.

Based off these results it seems that a prediction horizon with length $N = 15$ yield the most cost-effective operation of the NMPC. An argument could still be made to use $N = 5$ as it yield the most C. This may however come at the expense of more excessive input usage and overshooting. $N = 15$ is in the end the preferred length of the prediction horizon as it provides, unlike $N = 5$ accurate long-term predictability for the NMPC.

5 Conclusion and further work

Based off the results provided in Section 4, it is reasonable to conclude that the NMPC is functioning. The NMPC is able to maximise C by continuously increase the production of it while at the same time not violating the system constraints. All of the states, inputs and algebraic variables have smooth trajectories and display realistic behaviour. As illustrated by the results in Section 4.2, the length of the prediction horizon significantly affect the performance of the NMPC in the range $N = 0$ to $N = 15$. As discussed, a prediction horizon with length $N = 15$ appear to yield the most cost-effective operation of the NMPC, although the over-aggressive alternative, $N = 5$, yield more C. A further increase from $N = 15$ appear to yield almost identical trajectory regardless, something which indicate that there are no operational benefit of using a prediction horizon with a length greater than $N = 15$. This indicate that $N = 15$ results in a prediction horizon that is able to predict future states of the system accurately enough for optimal operation.

Originally, the plant model introduced in Equation 9 originates from an article (Thangavel et al. 2020) that investigates the robustness of a multi-stage NMPC using so-called Sigma points. In the article, the model parameters given in Equation 11 are actually uncertain parameters that is to be estimated in a branching tree scenario. To implement this parameter estimation was originally a goal of this project, but during the work period it was decided leave this topic out of scope and rather focus on designing a functional NMPC. Further work of this project could therefore be to somehow implement this parameter-estimation for the NMPC, thereby making the controller more accurate and applicable for online control.

Generally further work of this project could be to make the model more realistic. This could for instance be to implement a measurement noise filter, for instance a Kalman filter with a moving horizon estimator. The noise measured in the plant model given in Equation 9 has in this project not been accounted for and implementation of the Kalman filter would address this uncertainty. Other aspects could be to make the plant model more realistic by adding corrective terms which could address nonideal behaviour such as chemical mixing and temperature uniformity in the reactor.

Another topic that might be interesting to investigate could be to reconsider the procedure of solving the optimisation problem. For example the computational feasibility of utilising multiple shooting instead of orthogonal collocation could be explored. Investigating different settings of the IPOPT-solver, or even the choice of solver, could also yield different performance results.

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