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A new model predictive control strategy for a continuous stirred tank reactor

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Abstract

A continuous stirred tank reactor (CSTR) is a frequently used reactor in processing engineering. This reactor is normally operated at steady state and is assumed to be perfectly mixed. Within CSTR, the temperature, concentration, or reaction rate do not have time or position dependences. On the other hand, model predictive control (MPC) is a control strategy that can handle state and control multivariables at same time. In this work, we will use MPC to find the control strategy of an eight-state CSTR. In the MPC problem formulation, a nonlinear optimal control problem arises using a final-time performance index, the CSTR model as well as box constraints on the control variables. This optimal control problem is solved by a fast-direct method. For the CSTR states steadiness, additional auxiliary constraints are used. These auxiliary constraints are manipulated by linear parameters. Both auxiliary constraints and linear parameters are inserted to the optimal control problem formulation. That is, the solution of the optimal control problem includes these optimal parameters to ensure the CSTR state steadiness. Simulation results using IPOPT under C/C++ environment is presented to show the effectiveness of the proposed control strategy.

Keywords: Continuous stirred tank reactor, model predictive control, state stability.

1. Introduction

Chemical reactors are considered of the top important and attractive topics in chemical engineering not only for chemical engineers, but also for system engineers as well as mathematicians since these systems need complex mathematical tools to analyze them. One of these attractive mathematical sides of chemical reactors is the optimization or optimal control. The optimal control (or dynamic optimization) means that we need to find the optimal operating solution for the system depending on its mathematical model and such performance measure.

A nonlinear continuous stirred chemical reactor (CSTR) is also used as a proofing case study by many mathematicians and system engineers in the filed of optimal control research, for instance, Luss (Luss,1990) has used a non-linear system consisting of five simultaneous chemical reactions tanking place in an isothermal continuous stirred tank reactor, as first introduced by (Jensen, 1965) and revised by (Lapidus & Luus, 1967). He used this challenging CSTR system to test a dynamic programming algorithm that deals with high-dimensional nonlinear optimal control problems. Within this test, no difficulties were encountered in convergence to the optimal solution using several optimization iterations

Biegler with other scholars (e.g., (Biegler, Damiano, & Blau, 1986), (Lakshmanan, Rooney & Biegler, 1999), (Zavala & Biegler, 2006) and (Hoang, Barz, Merchan, Biegler & Arellano-Garcia, 2013)) have paid many efforts in developing optimization algorithms that target enhancing the computational expense of the direct solution of the

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optimal control problem or posing optimal control problem formulations that grantee the state stability. These algorithms are well tested using practical chemical engineering case studies such as CSTR.

In (de Oliveira Kothare & Morari, 2000) an optimal control problem formulation in the discrete system dynamics is presented and used in the model predictive control algorithm based on a contraction property of the state feedback control which guarantees stability of the system states while using a less restrictive additional constraint. Their method is well tested using an ideal nonlinear CSTR to show the closed-loop asymptotic stability. However, in (Qin & Badgwell, 1997 & 2003), one can find a "good" review of using the optimal control problem as well as model predictive control theories in chemical engineering.

In this paper we use a fast-direct optimal control problem solution that is firstly proposed by (Tamimi & Li, 2009) which is a combination between multiple shooting and collocation on finite element methods to solve a challenging isothermal-nonlinear CSTR system. For the CSTR state stability we use stabilizing (auxiliary constraint) added to the optimal control problem formulation to guarantee the state stability. In this formulation (Tamimi & Li, 2011), the systems state stability is ensured by introducing auxiliary state variables and corresponding linear state equations. The system states are enforced to be contracted with respect to the auxiliary state variables by adding inequality constraints. That is, the system states will be stable, if the auxiliary states are stable. The eigenvalues of the linear state equations introduced will be determined to stabilize the auxiliary state variables and at the same time make the optimal control problem feasible. This is achieved by considering the eigenvalues as optimization variables in the optimal control problem. Therefore, the solution of the optimal control problem guarantees the feasibility, stability and optimality of the NMPC system

The remaining section of this paper is organized as follows: Section 2 presents the model predictive control principle as well as the direct solution of the optimal control problem. Section 3 presents the used method for stabilizing the system states. A nonlinear CSTR case study is presented in Section 4 where paper conclusion comes in Section 5.

2. Model predictive control

Model predictive control (MPC) is a control strategy that was developed in the last five decades. The control prediction in this method lies on using the system model that represents the system dynamics and normally is written using a set of differential/ difference equations with initial conditions as well as some constraints on the systems states and controls. This is done by formulating an optimal control problem that is dedicated to optimizing (minimize or maximize) a pre-selected performance index, normally objective functional, along a prediction horizon subject to the system dynamics that are represented by differential or difference equations, as well as initial conditions of the states.

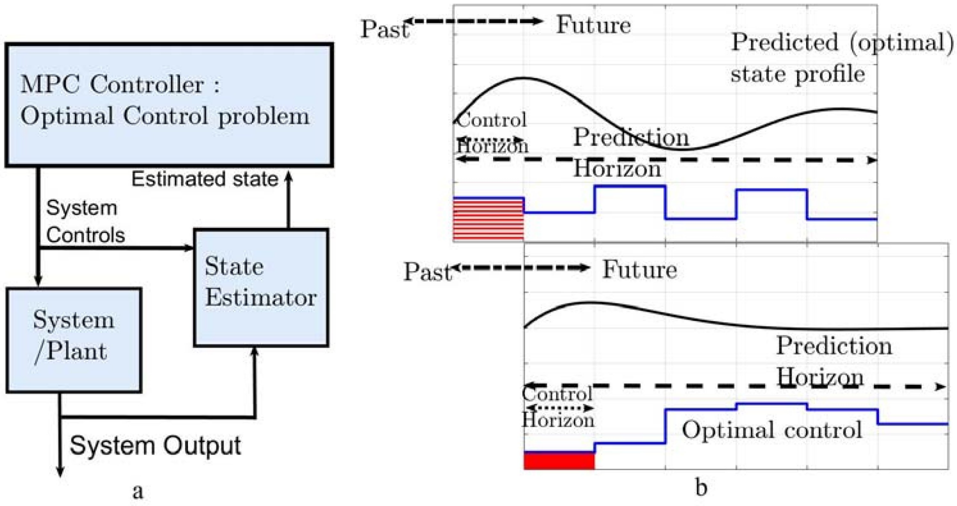

Figure1: a: Basic MPC structure, b: Principle of MPC

Theses initial conditions are normally measured or estimated by a dedicated sensor or estimator, respectively. The solution of the optimal control problem yields optimal control profiles with corresponding optimal (predicted) state profiles. The optimal controls will be easily sent to the system input; therefore, the system states are expected to follow the optimal (predicted) state profiles. If the system has no disturbances the system states and the predicted states must be identical If this is not the case, new readings or estimations must be available to re-solve the optimal control problem again on a new shifted prediction horizon then the new control results are sent again to the system and so on.

The time between two sensor readings or estimation, i.e. the sampling rate, is also known by the control horizon and the optimal control problem is solved each MPC step.

Figure 1a shows the basic structure of the MPC as it is applied in a closed-loop system while Figure 1b shows the basic principle of the MPC.

The optimal control problem of the MPC and its solution are the most important key-players in the MPC. Several methods have been proposed to solve the optimal control problem in the literature. However, these methods are grouped into three methods; dynamic programing, indirect methods and direct methods (Tamimi, 2011). In the direct method the optimal control is firstly discretized to transform it to a nonlinear programing (NLP) problem, and then this NLP is solved by one of the NLP-solvers such as sequential quadratic programing (SQP), sparse nonlinear optimizer (SNOPT) or interior point optimizer (IPOPT). In this paper, we use a direct method that is developed by (Tamimi & Li, 2011), namely, a combined multiple shooting with collocation on finite elements, to solve the optimal control problem. However, the optimal control problem that will be considered in this paper has the following formulation:

Find the control input profiles, $u(t)$, for the system that has the dynamics

$$\dot{x} = f\big(x(t), u(t)\big) \tag{1}$$

$$x(t_i) = x_i \tag{2}$$

that minimize the objective functional

$$\mathrm{J} = \int_{t_i}^{t_i+T} L(x(t), u(t), t)dt \tag{3}$$

and some box constraints

$$x_L \le x(t) \le x_U \tag{4}$$

$$u_L \le u(t) \le u_U \tag{5}$$

where vectors x(t)\inR$^{\mathrm{n_x}}$, and $u(t) \in R^{n_u}$ are the state vector and the control vector, respectively, $f\colon R^{n_x} \times R^{n_u} \rightarrow R^{n_x}$ and $J\colon R^{n_x} \times R^{n_u} \times R_+ \rightarrow R_+$are the system dynamics and the objective functional, respectively. T *and* t_i are the prediction time horizon and initial time instant, respectively, where the script i refers for the MPC step or the sampling instant.

Moreover, the combined multiple shooting with collocation on finite elements method that is used to solve the above optimal control problem can be summarized as follows:

- Divide the time horizon into N equal subintervals $\Delta T, where.$

$$t_i < t_i + \Delta T < t_i + 2\Delta T \ldots < t_i + N\Delta T = t_i + T \tag{6}$$

- Parameterize the control function in each subinterval by a vector z:

$$u_j(t) = u_j\big(t, z_j\big), t \in [t_i, t_i + j\Delta T], j = 1,2,..,N \tag{7}$$

- Parameterize the initial conditions of the states in each subinterval by a vector w

$$x_j\big(t_j\big) = w_j,\ j = 1,2,..,N \tag{8}$$

  Here the parameters z_j and w_j are box- constrained, that is:

$$x_L \le w_j \le x_U \text{ and } u_L \le z_j \le \mathrm{u_U} \tag{9}$$

- Calculate the state trajectories in each subinterval and the values of the states at the end of each subinterval using the parameterized values of the states at the beginning of each subinterval using collocation on finite elements, such that;

$$\mathrm{x}(t) = \sum_{j=0}^{M}\left(x_j\big(t_{jl}\big)\left(\prod_{l=0 l\neq j}^{M}\frac{t-t_{il}}{t_{ij}-t_{il}}\right)\right). \tag{10}$$

  where M is the number of collocation points in each element (subinterval).

- Define continuity constraints to maintain a continuity property of the states between the subintervals.
$$w_{j+1} - x_j\left(w_j, z_j, t_j\right) = 0 \qquad (11)$$
- Evaluate the objective function in each subinterval and formulate the NLP problem:
  Find the vectors $w_j, z_j, j = 1,2 \ldots, N$, that make the objective function $J = \sum_{j=1}^{N-1} L\left(w_j, z_j\right)$ minimum subject to the Equality constraints (11) and Inequalities (9).
- Find the NLP sensitivities; here the first order sensitivities is computed using the first Taylor expansion of the sensitivity equation:
$$\frac{\partial S}{\partial w_{ij}} + \frac{\partial S}{\partial w_{i0}} + \frac{\partial S}{\partial w_i} = 0 \qquad (12)$$
  where $S = x(t) - \sum_{j=0}^{M}\left(x_j\left(t_{jl}\right)\left(\prod_{l=0 l\neq j}^{M}\frac{t-t_{il}}{t_{ij}-t_{il}}\right)\right)$.
- Solve the NLP problem using the SQP method.
  Figure 2 gives an example of an optimal control problem which is initialized (to the left) and solved (terminated) after several iterations (to the right).

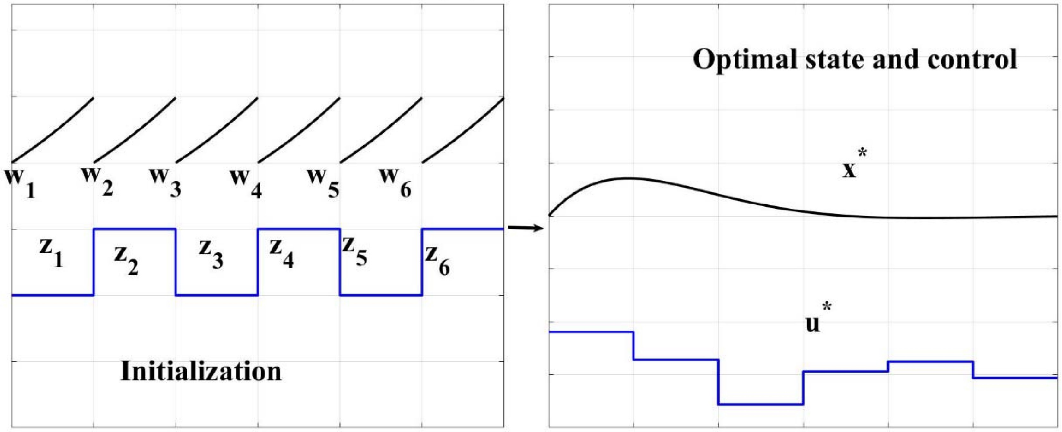

Figure 2: State and control profile in the first and final iterations using multiple shooting with collocation on finite element

3. Model predictive control stability constraints

The stability analysis of MPC schemes has long been a challenge due to several reasons such as nonlinear system dynamics and state constraints. Stability can be ensured by using stability constraints (besides the input and state constraints) by introducing, e.g., terminal equality constraints or terminal regional constraints in combination with terminal costs within the finite horizon optimization problem. However, such additional terminal constraints often significantly increase the online computational effort necessary to solve the open loop optimization problem and may cause feasibility problems. (de Oliveira Kothare & Morari, 2000) proposed an MPC (CNTMPC) algorithm based on a contraction property of the state feedback control which guarantees stability while using a less restrictive additional constraint.

In this study we use an MPC scheme in which the controlled system is rendered asymptotically stable by introducing time varying auxiliary state variables and coupling constraints. The concept of this method is much more flexible and does not require a costly preparation phase to adjust, e.g., a contraction parameter. Here, both the performance index, which is given by the integrated running costs, and the dynamics of the introduced auxiliary states are considered in the formulation of the optimal control problem. The latter is represented by a linear system and can, thus, be steered by adequately adjusting the respective eigenvalues. The option to adapt the eigenvalues in each optimal control problem is essential in order make it feasible. Since the eigenvalues are considered as optimization variables, feasibility, convergence, and optimality of the closed-loop system are gained through the solution of the optimal control problem. However, the optimal control problem formulation that will be used in this paper and will ensure the states stability can be summarized as follows.

Find the control inputs profiles as well as a negative parameter vector $a = [a_1, a_2, \dots, a_{n_x}] \leq -\underline{a}$ for the system that has the dynamics Eqs. (1-2), box Constraints (4-5) and

$$\dot{y}_i(t) = A_k y_i(t), \qquad t \in [t_i, t_i + T_P] \tag{12}$$

$$-y_i(t) \leq x(t) \leq y_i(t), \qquad t \in [t_i, t_i + T]. \tag{13}$$

that minimize the objective functional

$$\mathrm{J} = \int_{t_i}^{t_i+T} L(x(t), u(t), t) + |y_i(t)|_Q^2 dt \tag{14}$$

where the initial condition $\mathrm{y_i}(0) = \mathrm{e}^{\mathrm{A_i}\mathrm{i}(t_{i+1}-t_i)} y_0$, $A_i = diag([a_1, a_2, \dots, a_{n_x}])$.

Here $|\, y(t)_i \,|_Q^2 = y_i(t)^T Q y_i(t)$ is a weighted norm with positive semi-definite matrix $Q \in R^{n_x \times n_x}$ which can be selected offline. This means that a quadratic penalty term with a weighting penalty matrix Q is added to the objective function to penalize the auxiliary state in the optimization problem. If the coupling Constraint (13) is not active in the $i-th$ component of the predicted trajectory $x(t; \hat{x}, u)$ for any $t \in [t_i, t_i + T]$, the corresponding eigenvalue should be chosen smaller in order to reduce the influence of this penalty term on the objective function. On the other hand, if the penalty term of the objective function is omitted, the optimal eigenvalues are all equal to $-\underline{a}$.

Figure 3 shows an example that illustrates the behaviour of the closed-loop generated by the MPC method for an asymptotically stable perturbed system where the sampling time is $(t_{i+1} - t_i)$. The auxiliary state (red-dashed) enforces the system state (blue-solid) to decay exponentially in the first optimization step since the auxiliary state in the first optimization step satisfies $y_0 e^{A_i t}$. Although the initial conditions of the auxiliary state in two successive optimization steps are equal, e.g. the initial conditions for first and second $(k = 0{,}1)$ are always z_0 at $t = t_0$, the dynamic of the auxiliary states may not be equal $A_0 \neq A_1$, and the system state is enforced to be enveloped by the auxiliary state. When many optimization steps are done, say $(k > 100)$, the time constants of the auxiliary state in two successive optimization steps satisfy $A_i \cong A_{i+1}$. That means, when the MPC algorithm begins, the state decaying will be heavy, but when many optimization steps are done the system decaying will decrease as i increases.

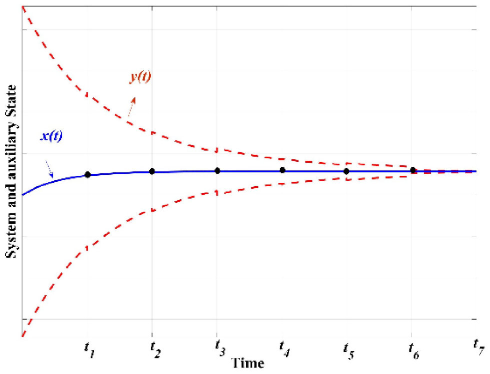

Figure 3: The auxiliary constraint action

4. Model predictive control of continuous stirred tank reactor

In this section, we consider a complex photochemical reaction in an isothermal CSTR, as formulated by (Jensen, 1965) and used for optimal control studies in (Luss, 1996) and (Park & Ramirez, 1988) The mechanism for the reactions among the species A, B, C, D, E, F and G is given by:

$$A + B \xrightarrow{k_1} 2D$$

$$C + B \xrightarrow{k_2} CB$$

$$CB + B \xrightarrow{k^*} 3E$$

$$E + D \xrightarrow{k_3} 2F$$

$$A + F \xrightarrow{k_4} 2G$$

where the fifth reaction is photochemical, and its rate is proportional to the square root of the light intensity. The intermediate compound CB is postulated to be present in immeasurably small quantities, so it satisfies the stationary condition, namely d(CB)/dt = 0. By using a convenient set of parameters, (Lapidus & Luus, 1967) showed that the system is described by the eight differential equations, the optimal control problem is then:

Find the inlet feed rate of pure components A, B and $C; u_1 u_2$ and u_4, respectively, as well as square root of light intensity u_3 of the CSTR dynamics:

$$\dot{x_1} = u_4 - qx_1 - 17.6x_1x_2 - 23x_1x_6u_3 \tag{15}$$

$$\dot{x_2} = u_1 - qx_2 - 17.6x_1x_2 - 146x_2x_3 \tag{16}$$

$$\dot{x_3} = u_2 - qx_3 - 73x_2x_3 \tag{17}$$

$$\dot{x_4} = -qx_4 + 35.2x_1x_2 - 51.3x_4x_5 \tag{18}$$

$$\dot{x_5} = -qx_5 + 219x_2x_3 - 51.3x_4x_5 \tag{19}$$

$$\dot{x_6} = -qx_6 + 102.6x_4x_5 - 23x_1x_6u_3 \tag{20}$$

$$\dot{x_7} = -qx_7 + 46x_1x_6u_3 \tag{21}$$

$$x(0) = [0.1883\ 0.2507\ 0.0467\ 0.0899\ 0.1804\ 0.1394\ 0.1046]^T \tag{22}$$

$$[0\ 0\ 0\ 0]^T \leq u(t) \leq [20\ 6\ 4\ 20]^T \tag{23}$$

where $x_1, x_2, \ldots, x_7$ are weight fractions of species $A, B, \ldots, G$, respectively, $k_1, \ldots, k_4$ are the reaction rate constants and $q = u_1 + u_2 + u_4$ is the total flow rate of inlet streams. At the same time the control $u(t)$ must minimize the objective functional (that represents the profit of the reactor):

$$\mathrm{J} = \int_0^{0.2} 5.8(qx_1 - u_4) - 3.7u_1 - 4.1u_2 + q(23x_4 + 11x_5 + 28x_6 + 35x_7) - 5u_3^2 - 0.09 \tag{24}$$

In this case study, we assume the prediction horizon is 0.2 hour and we pick the control horizon 0.04 hour. We divide the prediction horizon into ten subintervals, therefore, the control horizon counts two subintervals. That is the objective functional Eq. (24) can be rewritten as

$$\mathrm{J} = \int_{t_i}^{T+t_i} 5.8(qx_1 - u_4) - 3.7u_1 - 4.1u_2 + q(23x_4 + 11x_5 + 28x_6 + 35x_7) - 5u_3^2 - 0.09 \tag{25}$$

where T is 0.2 Hour and $t_i = 0,\ 0.04,\ 0.08,\ 0.12,\ 0.16 \ldots etc.$ If the MPC strategy is directly applied the state $(x_i, i = 1,2,..,7)$ and control $(u_i, i = 1,2,3, and\ 4)$ profiles are shown in Figure 4 in blue-dashed curves. However, if an Inequality (13) is added to the optimal control problem.

Figure 4 shows the CSTR control profiles; u_1, u_2, u_3 and u_4, and the CSTR state profiles; $x_1, \ldots, x_7$. These control and state trajectories are computed using two conditions; the first condition is without any auxiliary or stabilizing constraints and the final states' values are free. These trajectories are shown in Figure 4 with dashed-blue lines, However, the red-dolid trajectories represent the control and state profiles with using the auxiliary (stabilizing) constraints (cf. Eq. 13), and thus the final state condition must be preselected, in other words, the stationary state value must be determined offline. The computation is done over 24 MPC step. From these computations we see that the system state using stabilizing constraints will converge faster than the states without stabilizing constraint.

5. Conclusions

In this paper, a fast-direct solution of the optimal control problem is presented, namely, a combined multiple shooting with collocation on finite elements. This method merge both advantages of direct multiple shooting and collection methods. The original optimal control formulation is also re-studied, so that, one can ensure the state stability. In this formulation, the basic finite horizon optimization problem is augmented by (linear) auxiliary states which enforce stability of the original states using coupling constraints, in addition, the eigenvalues of the auxiliary state dynamics are considered as optimization variables besides original system controls. In addition, a nonlinear CSTR case study are used to test the effectiveness of the presented MPC.

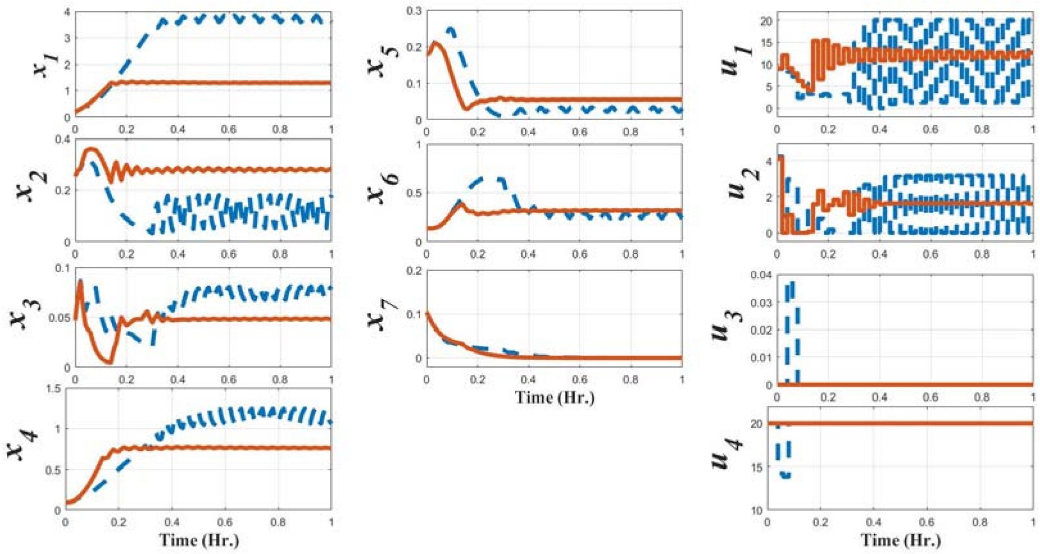

Figure 4: MPC Control and corresponding state profiles of the nonlinear CSTR using 24 MPC steps. Blue-dashed: without auxiliary constraints. Red-solid: with using auxiliary constraints.

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