APPLICATION OF AN INFINITE HORIZON MPC TO A NONLINEAR OPEN-LOOP UNSTABLE REACTOR SYSTEM

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ABSTRACT

A state space model for integrating and open-loop unstable systems is presented. The novel representation decomposes stable, unstable and integrating modes of the system, which in turn leads to the development of an infinite horizon MPC (IHMPC) for unstable systems. Equality constraints enforce that the system states corresponding to the integrating and unstable dynamics are zeroed whenever it is feasible. In this work, the control of a nonlinear CSTR with cooling jacket undergoing an exothermic irreversible reaction at an unstable steady state has been studied. The simulated results showed that the proposed IHMPC is capable of sustaining the system at its unstable steady state, rejecting unmeasured input disturbances and driving the system to a different steady state.

Keywords: model predictive control; nonlinear control.

1. INTRODUCTION

Model Predictive Control (MPC) is widely used in the chemical and petrochemical industries and is arguably the most advanced process control strategy to date (Garcia, Prett, & Morari, 1989). Its most interesting features are the capability to account for input, control moves and output constraints directly into the control problem, and its straightforward application to Multiple-Input and Multiple-Output (MIMO) systems. Although MPC applications to open-loop stable systems are far more common in the literature, some processes and configurations give rise to open-loop unstable systems. For instance, linearized models identified around nominal operating points of processes with recycle, mass and heat integration networks and reactions systems, such as Continuous Stirred Tank Reactors (CSTR) or batch reactors in which exothermic reactions are taking place, CSTR operating in cascade fashion, polymerization reactors, and so on. In particular, it might be sought to operate a reactor system at its unstable point for economic reasons (Gobin, Zullo, & Calvet, 1994; Özkan & Çamurdan, 1998). In this fashion, some effort has been put on the development of control strategies for open-loop unstable systems.

Several attempts to control open-loop unstable systems have been reported in the literature. The first attempts to control such systems were done employing classic PI or PID controllers, and even though these strategies are easy to implement and yield satisfactory results for stable systems, poor performance lead to the development of alternative control strategies. (Lee, Lee, & Park, 2000). Liu, Zhang, & Gu (2005) identified the two major limitations of PID control of open-loop unstable systems as excessive overshoot and large settling time in setpoint tracking scenarios. The authors developed a two degrees of freedom (2DF) control approach, comprised of three control blocks: the first one is a proportional-only controller that stabilizes the unstable system, and the second and third blocks decouple setpoint tracking and load disturbances effects control performance. Robust stability on is demonstrated via the Small-Gain Theorem for multiplicative model uncertainty, and simulation results showed that the proposed technique performs better than classic PID control regarding both overshoot and settling time problems. Huang & Chen (1997) put forward a formal demonstration of the PID limitations open-loop unstable set-point tracking and on disturbance rejection performance observed in Liu et al. (2005), and developed a 2DF control framework capable of suppressing overshoot for both first and second order unstable processes.

It was proposed by Rotstein & Lewin (1992) an adaptive tuning algorithm for PID controllers, which takes advantage of a real-time pole placement algorithm to select the most appropriate PID controller structure. A case study depicting the control of an exothermic reaction in a batch reactor showed that. counterintuitively, the adaptive PID strategy is not always better than the classic PID approach. The proposed control strategies for open-loop unstable systems up to here are mostly limited for applications in SISO systems.

Gobin et al. (1994) controlled a styrene polymerization reaction in a two-CSTR cascade system with a Dynamic Matrix Control (DMC) algorithm. The step response coefficients were obtained from a linearized model identified at a stable operating point, and the authors reported that their approach is faster than classic PID controllers in setpoint tracking scenarios. However, it is known that such process is highly non-linear, and the reported DMC approach is limited to a restricted operating region.

Hidalgo & Brosilow (1990) developed a coordinated MPC framework, in which the control actions, for each input, are independently calculated. The control framework was applied to a free radical solution polymerization of styrene in a CSTR. The authors stated that safe control of unstable processes is only feasible when there are sufficient degrees of freedom to keep the process within a small region about the desired operating point, therefore, MIMO layouts are essential. A simulation example showed that the proposed strategy stabilized the CSTR at its unstable operating point.

A cascade control structure for open-loop unstable processes was proposed in Özkan & Çamurdan, (1998). First, a proportional-only controller stabilizes the system, then, a linearized model is identified at the stabilized operating condition, and its step response coefficients are used to design a DMC. The authors verified that once the unstable system is stabilized, the resulting control problem is trivial, and real time calculation of the DMC model, at each time step, does not improve control performance.

Demircan, Camurdan, & Postlethwaite (1999) developed a DMC based on a fuzzy relational model for open-loop unstable systems. The advantages over the classic step response coefficients model are: it is an alternative for costly and knowledge demanding firstprinciple model; and it represents the process accurately over a large operating range, even though the model is identified from data obtained in a limited range. The results showed that such model works well for processes with unusual dynamic behavior. The control strategies listed previously were based, to some extent, on the DMC control strategy, and alternatives to mitigate the limitations of modeling an unstable process as an input-output step response.

Muske & Rawlings (1993) developed a nominally stabilizing MPC based on a state-space model for open-loop stable and unstable systems. Equality constraints

were enforced upon the states that represent the unstable dynamics of the systems, to guarantee that such states are zeroed after the control horizon. It was shown that in case of incomplete state measurement, a stable observer and a constrained regulator guarantee a nominally stabilizing controller.

The control approach for open-loop unstable and integrating systems proposed here is based on an extension of the state-space model presented in Santoro & Odloak (2012). The redefinition of system states to accommodate the unstable dynamics is shown in Section 3, and the IHMPC for integrating and open-loop unstable systems is proposed in Section 4. It is presented a case study to illustrate the proposed approach, and for this end an exothermic irreversible reaction in a nonlinear CSTR with cooling jacket system is analyzed. Results and discussions are given in Section 5. Finally, conclusions and suggestions for future works are presented in Section 6.

2. STATE SPACE MODEL REPRESENTATION FOR OPEN-LOOP UNSTABLE PROCESSES

The state-space model for unstable systems proposed here is an extension of the state-space model for integrating and time delayed systems developed in Santoro & Odloak (2012). The original work arranges the system model matrices, separate three types of states: those related to the stable modes, the original integrating modes and finally the integrating states derived from the velocity representation. The extension of the proposed formulation includes the unstable states as well.

Considering a system with ny outputs and nu inputs, the transfer function relating input u_i and output y_i is

$$G_{i,j}(s) = \frac{(b_{i,j,0} + b_{i,j,1}s + \dots + b_{i,j,nb}s^{nb})}{s(s - r_{i,j,1}) \cdots (s - r_{i,j,na'})(s - r_{i,j,1}^{um}) \cdots (s - r_{i,j,nun}^{um})}$$
(1)

where {*na'*, *nb*, *nun* \in *N* | *nb* < *na'*+*nun*}, *na'* is the number of stable poles and *nun* is the number of unstable poles, and $r_{i,j,1},...,r_{i,j,na'}$ are the distinct stable poles and $r_{i,j,1}^{um},...,r_{i,j,nun}^{um}$ are the distinct unstable poles of the system. Then, for a sampling period Δt , the corresponding step response at time step *k* can be computed by the expression:

$$S_{i,j}(k) = \begin{pmatrix} d_{i,j}^{0} + d_{i,j,l}^{d} e^{r_{i,j,k} \Delta t} + \dots + d_{i,j,na'}^{d} e^{r_{i,j,na'} \Delta t} \\ + d_{i,j,l}^{dun} e^{r_{i,j,k}^{m} \Delta t} + \dots + d_{i,j,num}^{dun} e^{r_{i,j,num}^{m} \Delta t} + d_{i,j}^{i} k \Delta t \end{pmatrix} (2)$$

in which the coefficients $d_{i,j}^0, d_{i,j,1}^d, ..., d_{i,j,na'}^d, d_{i,j,1}^{dum}, ..., d_{i,j,nun}^{dum}$ and $d_{i,j}^i$ are obtained from the partial fractions expansion of the transfer function $G_{i,j}(s)$ Then, the following state-space model is defined:

$$x(k+1) = Ax(k) + B\Delta u(k)$$

$$y(k) = Cx(k)$$
(3)

$$\begin{aligned} x(k) &= \left[x^{s}(k)^{T} \quad x^{d}(k)^{T} \quad x^{m}(k)^{T} \quad x^{i}(k)^{T} \quad x^{i}(k)^{T} \right]^{T}, \\ x \in \mathbb{C}^{nx}, x^{s} \in \mathbb{R}^{ny}, x^{d} \in \mathbb{C}^{nd}, x^{i} \in \mathbb{R}^{ny}, x^{m} \in \mathbb{C}^{man}, y \in \mathbb{R}^{ny}, \\ nx &= 2ny + nd + nun, \qquad nd = ny.nu.na', \qquad \text{and} \\ A &= \begin{bmatrix} I_{ny} & 0_{ny \times nd} & 0_{ny \times nun} & \Delta tI_{ny} \\ 0_{nd \times ny} & F & 0_{nd \times nun} & 0_{nd \times ny} \\ 0_{nm \times ny} & 0_{nm \times nd} & F_{un} & 0_{nm \times ny} \\ 0_{nm \times ny} & 0_{nm \times nd} & 0_{ny \times nun} & I_{ny} \end{bmatrix} \end{bmatrix}, \qquad A \in \mathbb{C}^{nx \times nx}, \\ B &= \begin{bmatrix} B^{s} \\ B^{d} \\ B^{m} \\ B^{i} \end{bmatrix}, \qquad B \in \mathbb{C}^{nx \times nu} \\ B^{s} &= D^{0} + \Delta tB^{i}, \qquad B^{d} = D^{d}FN, \qquad B^{im} = D^{dm}F_{un} \\ B^{i} &= \begin{bmatrix} d^{i}_{1,1} & \cdots & d^{i}_{1,ny} \\ \vdots & \ddots & \vdots \\ d^{i}_{ny,1} & \cdots & d^{i}_{ny,ny} \end{bmatrix}, \qquad B^{i} \in \mathbb{R}^{ny \times nu}, \\ D^{0} &= \begin{bmatrix} d^{0}_{1,1} & \cdots & d^{0}_{ny,ny} \\ \vdots & \ddots & \vdots \\ d^{0}_{ny,1} & \cdots & d^{0}_{ny,ny} \end{bmatrix}, \qquad D^{0} \in \mathbb{R}^{ny \times nu} \\ F &= \operatorname{diag} \begin{pmatrix} e^{\Delta r_{1,1,1}} & \cdots & e^{\Delta r_{1,1,nu'}} & \cdots & e^{\Delta r_{1,m,1}} & \cdots & e^{\Delta r_{1,m,nu'}} \\ \cdots & e^{\Delta r_{ny,1,nu'}} & \cdots & e^{\Delta r_{ny,m,1}} & \cdots & e^{\Delta r_{ny,m,nu'}} \end{pmatrix} \\ F &\in \mathbb{C}^{nd \times nd} \\ F^{im} &= \operatorname{diag} \begin{pmatrix} e^{\Delta r_{1,1,1}} & \cdots & e^{\Delta r_{1,1,nu'}} & \cdots & e^{\Delta r_{1,m,1}} & \cdots & e^{\Delta r_{ny,m,mu'}} \\ \cdots & e^{\Delta r_{ny,1,nu'}} & \cdots & e^{\Delta r_{ny,m,nu'}} & \cdots & e^{\Delta r_{ny,m,mu'}} \end{pmatrix} \\ F^{im} &= \operatorname{diag} \begin{pmatrix} d^{d}_{1,1} & \cdots & d^{d}_{1,nu} & \cdots & d^{d}_{1,nu,1} & \cdots & d^{d}_{nr,m,nu'} \\ \cdots & e^{\Delta r_{ny,1,nu'}} & \cdots & e^{\Delta r_{ny,m,nu'}} & \cdots & e^{\Delta r_{ny,m,mu'}} \end{pmatrix} \end{pmatrix}, \\ D^{d} &= \operatorname{C}^{nd \times nd} \end{aligned}$$

 I_n and 0_n are the identity and null matrices of dimension n, respectively. The reader is referred to the original formulation (Santoro & Odloak, 2012) for detailed explanation about the integrating states.

3. INFINITE HORIZON MPC FOR OPEN-LOOP UNSTABLE PROCESSES

The equations below define the IHMPC proposed here.

Problem 1

$$\min_{\Delta u(k+j|k),\delta_{y,k},\delta_{i,k},\delta_{im,k}} V_{1,k} \\
V_{1,k} = \sum_{j=1}^{\infty} \left\| y(k+j|k) - y^{sp} - \delta_{y,k} - (j-m)\Delta t \delta_{i,k} \right\|_{Q_{y}}^{2} \\
+ \sum_{j=0}^{m-1} \left\| \Delta u(k+j|k) \right\|_{R}^{2} + \left\| \delta_{y,k} \right\|_{S_{y}}^{2} + \left\| \delta_{i,k} \right\|_{S_{i}}^{2} + \left\| \delta_{um,k} \right\|_{S_{um}}^{2}$$
(4)

subject to (3) and

$$x^{s}(k+m|k) - y_{sp,k} - \delta_{y,k} = 0$$
(5)

$$x_{0}^{i}(k+m \mid k) - \delta_{ik} = 0$$
(6)

$$x^{un}(k+m) - \delta_{unk} = 0 \tag{7}$$

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$$\Delta u(k+j \mid k) \in U, \ j = 0, 1, ..., m-1$$

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$$U = \begin{cases} -\Delta u_{\max} \le \Delta u \ (k+j \mid k) \le \Delta u_{\max} \\ \Delta u \ (k+j \mid k) = 0, j \ge m \\ u_{\min} \le u(k-1) + \sum_{i=0}^{j} \Delta u(k+i \mid k) \le u_{\max} \end{cases}$$
(8)

where $Q_y \in \mathbb{R}^{ny \times ny}$, $Q_u \in \mathbb{R}^{nu \times nu}$ and $R \in \mathbb{R}^{nu \times nu}$ are positive semidefinite matrices; y(k+j|k) is the output prediction at time step k+j computed at time step kincluding the effects of the future control actions; $y_{sp,k}$ is the output reference; $\Delta u(k+j|k)$ is the input move $(\Delta u(k+j)=0, j>m)$. Moreover, $\delta_{y,k} \in \mathbb{R}^{ny}$, $\delta_{u,k} \in \mathbb{R}^{nu}$, $\delta_{i,k} \in \mathbb{R}^{ny}$, and $\delta_{un,k} \in \mathbb{R}^{num}$ are the slack variables that are introduced in the control problem in order to render the control problem always feasible, while $S_y \in \mathbb{R}^{ny \times ny}$, $S_u \in \mathbb{R}^{nu \times nu}$, $S_i \in \mathbb{R}^{ny \times ny}$, and $S_{un} \in \mathbb{R}^{nun \times num}$ are positive

 $S_u \in \mathbb{R}^{n}$, $S_i \in \mathbb{R}^{n}$, and $S_{un} \in \mathbb{R}^{n}$ are positive definite weighting matrices associated with these slacks.

The constraint defined in (7) tries to enforce that the unstable states will be zeroed at time step k+m. A suitable selection of the weighting matrix S_{un} makes the control problem converge in practical situations. However, a formal nominal stability demonstration is not provided here and is a subject for future works.

4. CONTROL OF A NON-LINEAR CSTR AT ITS UNSTABLE OPERATING POINT

It is studied the control of a CSTR with cooling jacket where an elementary irreversible reaction takes place (A \rightarrow B). It is assumed that the physical properties and heat transfer coefficient are constant; therefore the firstprinciples model that represents the true plant is given by the following set of nonlinear equations (Henson & Seborg, 1997):

$$\frac{dh(t)}{dt} = \frac{F_m(t) - F_{out}(t)}{\pi r^2}
\frac{dc_A(t)}{dt} = \frac{[c_{A,m} - c_A(t)]F_m(t)}{\pi r^2 h(t)} - k_0 \exp\left[-\frac{E}{RT(t)}\right] c_A(t)
\frac{dT(t)}{dt} = \frac{[T_m - T(t)]F_m(t)}{\pi r^2 h(t)} + \frac{-\Delta H}{\rho C_p} k_0 \exp\left[-\frac{E}{RT(t)}\right] c_A(t) + \frac{2U}{\rho r C_p} [T_c(t) - T(t)]$$
(9)

The parameters associated with this system are given in Table 1. In the 3x3 control structure considered here, the controlled outputs are the liquid level in the reactor $y_1 [h (m)]$, the reactant concentration $y_2 [c_A (\text{kmol/m}^3)]$ and the reaction temperature $y_3 [T (\text{K})]$. The manipulated inputs are the inlet flow rate $u_1 [F_{in}$

(m³/min)], the outlet flow rate $u_2 [F_{out} (m^3/min)]$ and the cooling fluid temperature $u_3 [T_c (K)]$.

Table 1: Nominal parameters of the CSTR system.		
Description	Values	
$c_{A,in}$ (reactant concentration in feed stream)	1.0 kmol·m ⁻³	
T_{in} (temperature in feed stream)	350 K	
r (radius of the reactor)	0.47 m	
k_0 (pre-exponential factor)	$6 \times 10^{10} \text{ min}^{-1}$	
<i>E/R</i> (activation energy/universal gas constant)	8,890 K	
U (overall heat transfer coefficient)	$315.6 \text{ W} \cdot \text{m}^{-2} \cdot \text{K}^{-1}$	
ρ (density of the reaction mixture)	$7 \times 10^2 \text{ kg} \cdot \text{m}^{-3}$	
C_p (heat capacity of the reaction mixture)	220 J·kg ⁻¹ ·K ⁻¹	
ΔH (enthalpy of reaction)	$-2 \times 10^7 \text{ J} \cdot \text{kmol}^{-1}$	

An unstable steady state was identified solving (9) when the left hand side equals zero and the process parameters are taken from Table 1. Model equations may be linearized around this unstable steady state, resulting in the transfer function model (10).

$$G(s) = \begin{bmatrix} \frac{1.44}{s} & \frac{-1.44}{s} & 0\\ \frac{0.44s^2 - 1.45s + 1.17}{s^3 + 0.17s^2 - 1.55s} & \frac{0.64s - 1.17}{s^3 + 0.17s^2 - 1.55s} & \frac{-0.02}{s^2 + 0.17s - 1.55}\\ \frac{-0.6s^2 + 32.13s - 46.19}{s^3 + 0.17s^2 - 1.55s} & \frac{-0.08s + 46.19}{s^3 + 0.17s^2 - 1.55s} & \frac{0.52s + 1.05}{s^2 + 0.17s - 1.55} \end{bmatrix}$$
(10)

The control problem defined in Problem 1 was solved in GAMS®23.6. The plant was simulated using the *ode45* algorithm in MATLAB®2010a. It was assumed that the model states are corrected by a steady-state Kalman filter, based on the deviation between the output values calculated by the state-space model (3) and the values calculated by the first-principle model (9). The IHMPC and Kalman filter tuning parameters employed in the case study are listed in Table 2.

The scenario analyzed here investigates if the IHMPC based on the proposed state-space model can keep the CSTR process at its unstable operating point. In this fashion, a simulation in which the system starts from $y_0 = [0.91 \ 0.82 \ 349.54]^{\mathrm{T}}$ and $u_0 = [0.91 \ 0.91 \ 250]^{\mathrm{T}}$ and it is driven towards the unstable steady state defined by the output values $y_{l}^{sp} = [0.91 \ 0.72 \ 350.03]^{T}$ is proposed. Once the system is stabilized, unmeasured impulse disturbances with intensity 5K and 0.25 m³/min affect inputs u₃ and u₂ at time instants 25min and 40min, respectively. Finally, the system is subject to a new setpoint, different from the unstable steady state: $y^{sp}_2 = [0.91 \quad 0.72 \quad 345.03]^{T}$. The input upper and lower bounds and control moves maximum values are $u_{min} = [0.01 \ 0.01 \ 200]^{\mathrm{T}}, u_{max} = [2 \ 2 \ 415]^{\mathrm{T}}, \text{ and} \Delta u_{max} = [0.065 \ 0.065 \ 15]^{\mathrm{T}}$ respectively. All the variable values defined here follow the units previously defined.

Table 2: IHMPC and Kalman filter tuning parameters.

Parameter		Value	
IHMPC			
Q_{v}		diag($[10^2 5 \times 10^6 10^4]$)	
$\tilde{Q_i}$		diag($[10^2 5 \times 10^6 10^4]$)	
S_{ν}		diag($[10^6 \ 10^8 \ 10^4]$)	
S_i		diag([10 10 1])	
S_{un}		diag($[10^4 \ 10^4 \ 10^4]$)	
R		diag($[10^{-2} \ 10^{-2} \ 10^{3}]$)	
т		7	
Δt		0.1 min	
Kalman Filter			
Process	noise	$10^3 \times I_{nx}$	
covariance matrix			
Measurement	noise	diag($[10^{-4} \ 10^{-4} \ 10^{-9}]$)	
covariance matrix			

Figures 1 to 4 depict the output and input responses of the system, the control cost function value, and the absolute value of the maximum component of the vector δ_{un} as a function of the simulation time, respectively.

It is observed that the IHMPC stabilizes the nonlinear CSTR at its unstable operating point in less than 20 minutes. The behavior of the cost function value and the absolute value of the maximum unstable slack variable indicate that the contribution of the setpoint deviation of y_3 affects the cost function the most. In fact, its weight in the cost function $(q_{y,3})$ and its respective δ_y weight were chosen as large values because this variable can easily lead to instability. It is also observed that the impact of the feed flowrate and cooling jacket disturbances are similar on y_1 , whereas the impact of the cooling jacket temperature disturbance is larger on y_2 and y_3 . Figure 2 shows that the feed flowrate disturbance is rejected in about 5 minutes, whereas the cooling jacket temperature disturbance rejection takes twice as long. The dot-dashed curves in Figure 1 depict the system outputs related to the estimated states . The largest deviations from the plant values, shown as continuous lines are observed for variable y_1 , especially regarding the oscillatory behavior amplitude, and in y_2 , from time instants 40 min to 45 min. It indicates that the tuning parameters of the Kalman filter were well chosen, and that the linearized model was capable to accurately represent the estimated states of the plant within the operating region. Finally, it is observed that the control cost function is not a monotonically decreasing function, nonetheless, in the present simulation the unstable slacks are zeroed and the control cost converges to zero. The setpoint change at 50 min drives the system further from the region in which the linearized model represents the nonlinear system well. Nonetheless, it is observed that the amplitude of the initial peak at 50 min, in Figures 3 and 4 decreases to a constant value within two minutes, and, from that time until the end of the simulation, all the system inputs and outputs oscillate. The trend observed in Figure 4, which depicts the absolute maximum value of the unstable slacks vector, is similar to the one in Figure 3. It indicates that there is a heavy contribution of the unstable slacks to the control cost function. Moreover, it is noted from time instants 25 to 30, 40 to 45 and 55 until the end of the simulation that the cost function of the controller proposed here is not a Lyapunov function, therefore asymptotic stability of the closed-loop is not demonstrated here.

The sampling time interval Δt =0.1 min was necessary to adequately deal with the mismatch between the nonlinear plant and the linearized model is the simulation considered here. Nonetheless, since it is merely a QP, it is reasonable to assume that Problem 1 is solvable in less than 6 seconds, and the optimum control actions are readily available.



Figure 1: Simulated output responses.







Figure 4: Maximum absolute entry of the vector of unstable slack variables, δ_{un} .

5. CONCLUSIONS

A state-space model based on the analytical stepresponse of the system was used to formulate an IHMPC for stable, integrating and unstable systems. The latter may arise from operating processes at unstable regions for optimum profit, for example. It is shown in a simulated case study that the proposed framework is successfully capable of controlling an exothermal irreversible reaction in a nonlinear CSTR with cooling jacket at its unstable steady state. Moreover, input disturbance rejection capabilities were observed. However, oscillatory behavior was present when the process was operating far from the region in which the linear model of the IHMPC was identified.

The work presented here does not provide formal stability guarantees, although the simulation shows that an appropriate selection of the IHMPC and Kalman filter tuning parameters can stabilize the closed-loop system as long as no constraints are violated. A formal stability demonstration, and the extension of the algorithm to account for multi-plant uncertainty are intended topics for future works.

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