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Economic NMPC Strategies for Solid Sorbent-Based CO_2 Capture

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Abstract: Nonlinear Model Predictive Control (NMPC) enables the incorporation of detailed dynamic process models for nonlinear, multivariable control with constraints. This optimization-based framework also leads to on-line dynamic optimization with performance-based and so-called economic objectives. Nevertheless, economic NMPC (eNMPC) still requires careful formulation of the nonlinear programming (NLP) subproblem to guarantee stability. In this study, we derive a novel reduced regularization approach for eNMPC with stability guarantees. The resulting eNMPC framework is applied to a challenging nonlinear CO_2 capture model, where bubbling fluidized bed models comprise a solid-sorbent post-combustion carbon capture system. Our results indicate the benefits of this improved eNMPC approach over tracking to the setpoint, and better stability over eNMPC without regularization.

Keywords: nonlinear model predictive control, economic NMPC, bubbling fluidized bed, CO_2 capture, nonlinear optimization

1. INTRODUCTION

Model Predictive Control (MPC) is widely accepted in the process industries as a generic multivariable controller with constraint handling. It also extends to Nonlinear Model Predictive Control (NMPC) in order to realize high-performance control of highly nonlinear processes. NMPC allows incorporation of detailed process models (validated by off-line analysis) and integrates with on-line optimization strategies consistent with higher-level tasks, including scheduling and planning. NMPC for tracking and so-called "economic" stage costs, as well as associated state estimation tasks, have been reviewed, formulated and analyzed in considerable detail (Rawlings and Mayne (2009); Mayne et al. (2000)). Fundamental stability and robustness properties of NMPC are well-known, and many of the key issues related to the applicability and relevance of NMPC are well understood. Moreover, through proper formulations of the NMPC subproblem, stability and sensitivity properties of nonlinear programs (NLPs) are realized, leading to nominal and robust stability of the NMPC controller through input to state stability (ISS) (see Magni and Scattolini (2007); Yang et al. (2015)). Moreover, the existence of NLP solutions that are differentiable with respect to problem data leads to the development of sensitivity-based NMPC, which greatly reduces on-line computation and computational delay (Jäschke et al. (2014); Biegler et al. (2015)).

Setpoint-tracking NMPC can be readily extended to Economic NMPC through substitution of tracking stage costs by performance-based costs. On the other hand, economic stage costs are generally not $\mathcal{K}$ functions (see Definition 1) and therefore do not satisfy the assumptions needed for a Lyapunov-based stability analysis. As a result, advanced formulations of the NLP subproblem are required to realize stability and robustness properties. These are reviewed below and a novel extension of this approach is developed in this study and demonstrated for the dynamic real-time optimization of a CO_2 capture unit consisting of two bubbling fluidized bed (BFB) reactors.

The next section introduces NLP-based strategies for economic NMPC and provides background properties for the NLP subproblem. In particular, we describe the regularization of economic stage costs, which lead to nominal and robust (i.e., input to state stable (ISS)) stability. Section 3 develops a novel regularization scheme that leads to less conservative eNMPC controllers that still retain stability properties. This new eNMPC controller is demonstrated and compared on a challenging BFB model for carbon capture in Section 4. Finally, Section 5 concludes the paper and outlines directions for future work.

2. ECONOMIC NMPC WITH STAGE COST REGULARIZATION

We consider the following steady state optimization problem for economic NMPC with x_s and u_s as optimal steady state solutions.

$$\min_{x,u} \psi^{ec}(x,u) \text{ s.t. } x = f(x,u), u \in \mathbb{U}, x \in \mathbb{X}. \tag{1}$$

The dynamic optimization problem for economic NMPC is defined as follows:

$$\begin{aligned} V(x(k)) = \min_{v_l, z_l} \sum_{l=0}^{N-1} \psi^{ec}(z_l, v_l) \quad (2)\\ \text{s.t.} \quad z_{l+1} = f(z_l, v_l), l = 0, \dots N-1\\ z_0 = x(k), z_N = x_s\\ v_l \in \mathbb{U}, z_l \in \mathbb{X}. \end{aligned}$$

where the stage cost is given by $\psi^{ec}(\cdot,\cdot) : \Re^{n_x+n_u} \to \Re$ and is assumed to be Lipschitz continuous. For simplicity, we use an NMPC formulation with terminal equality constraints that incorporate the steady state optimum (x_s, u_s), instead of the origin.

Definition 1. (Magni and Scattolini (2007)) A continuous function $\alpha(.)$: $\Re_{\geq 0} \mapsto \Re_{\geq 0}$ is a $\mathcal{K}$ function if $\alpha(0) = 0, \alpha(s) > 0, \forall s > 0$ and it is strictly increasing.

Our stability analysis follows the Lyapunov stability framework where we derive the following inequality with the standard assumptions for setpoint tracking NMPC:

$$V(x(k+1)) - V(x(k)) \leq -(\psi(x(k),u(k)) - \psi(x_s,u_s)) \quad (3)$$

For economic NMPC, the economic stage cost $\psi^{ec}(x,u)$ can have an arbitrary form that represents the economic information for process operation. For an arbitrary economic stage cost, (3) does not apply if ψ is not a $\mathscr{K}$ function. Under these conditions, the value function for economic NMPC cannot be used as a Lyapunov function for stability of the closed-loop system.

To guarantee stability of economic NMPC, additional properties are needed. As shown in Angeli et al. (2012), dissipativity can be used to establish the stability for economic NMPC.

Definition 2. (Angeli et al. (2012)) A control system $x^+ = f(x,u)$ is dissipative with respect to a supply rate $s : \mathbb{X} \times \mathbb{U} \to \mathbb{R}$ if there exists a function $\hat{\lambda} : \mathbb{X} \to \mathbb{R}$, such that $\hat{\lambda}(f(x,u)) - \hat{\lambda}(x) \leq s(x,u)$ for all feasible control-input pairs. If in addition $\zeta : \mathbb{X} \to \mathbb{R}_{\geq 0}$ a positive definite function ($\zeta(x_s) = 0$ and $\zeta(x) > 0$ for all $x \neq x_s$) exists such that $\hat{\lambda}(f(x,u)) - \hat{\lambda}(x) \leq -\zeta(x) + s(x,u)$ then the system is said to be strictly dissipative.

By choosing the function $\hat{\lambda}(x) = \bar{\lambda}^T x$ for some $\bar{\lambda} \in \mathbb{R}^n$, the dissipativity assumption is equivalent to the following:

$$\min_{x,u} \quad \psi^{ec}(x,u) + \bar{\lambda}^T(x - f(x,u)) \geq \psi^{ec}(x_s,u_s) \quad (4)$$

As pointed out in Angeli et al. (2012), this assumption holds if the economic stage cost and dynamic model form a strongly dual problem. This also leads to the concept of rotated stage cost (Diehl et al. (2011); Angeli et al. (2012)) defined as follows:

$$\phi(x,u) = \psi^{ec}(x,u) + \lambda^T(x - f(x,u)) \quad (5)$$

where λ is the multiplier vector from the equality constraints in (1). Moreover, if the rotated stage cost $\phi(x,u)$ is strongly convex, then strong duality together with the stability of the corresponding economic NMPC can be guaranteed (Huang et al. (2011); Jäschke et al. (2014)). Their results provide sufficient conditions to establish stability for economic NMPC.

When strong convexity does not hold for $\psi^{ec}(x,u)$, an easy remedy is to add quadratic regularization terms to the economic stage cost. After introducing the regularization terms, the modified steady state problem and the corresponding regularized rotated stage cost are defined as follows:

$$\begin{aligned} \min_{x,u} \ & \psi^{ec}(x,u) + \frac{1}{2}\|(x,u) - (x_s,u_s)\|_Q^2 \\ \text{s.t.} \quad & x = f(x,u), u \in \mathbb{U}, x \in \mathbb{X}. \end{aligned} \quad (6)$$

with $\phi_{reg}(x,u) = \phi(x,u) + \frac{1}{2}\|(x,u) - (x_s,u_s)\|_Q^2$ where (x_s,u_s) are the optimal solutions of (1) and Q is a diagonal regularization weighting matrix. As shown in Jäschke et al. (2014), stability of the economic NMPC controller can be realized through the following procedure. First, we consider the *rotated* controller with rotated stage cost $\phi(x,u)$ as the objective function. With a sufficiently large regularization matrix Q, the regularized rotated stage cost $\phi_{reg}(x,u)$ becomes strongly convex (Jäschke et al. (2014)) and the local solution of (6) becomes a global minimum with the regularized rotated stage cost. With this result, the value function of this rotated controller decreases monotonically based on inequality (3) and leads to asymptotic stability. Moreover, since the economic NMPC controller has the same solution as the *rotated* controller, stability of regularized economic NMPC follows directly.

While adding regularization terms is easy, finding appropriate regularization weights that guarantee the stability of economic NMPC is challenging. In Jäschke et al. (2014), a systematic approach based on Gershgorin's theorem was proposed to find regularization weights for $Q = diag(q)$ that lead to strongly convex rotated stage costs $\phi_{reg}(x,u)$. These weights satisfy:

$$q_i > \sum_{i \neq j} |h_{i,j}| - h_{i,i} \quad (7)$$

where $h_{i,j}$ are the elements of the Hessian matrix of the rotated stage cost $\phi(x,u)$ in (5). Based on this simple criterion, we can determine the sufficient regularization weights that guarantee stability of economic NMPC. However, condition (7) must be checked and satisfied for all $u \in \mathbb{U}, x \in \mathbb{X}$ in order to guarantee that the regularized rotated stage cost is strongly convex. Biegler et al. (2015) grid the feasible regions for every variable, including differential states, algebraic variables and controls, and calculate the Hessian matrix of the rotated stage cost at each grid point. Though all calculations are done offline, they can be cumbersome, especially as the required number of calculations for (7) increases exponentially with problem size. Moreover, with this approach, regularization may be required for most system variables (i.e., dynamic states, algebraic variables and controls), and this could lead to very conservative economic performance.

To overcome this issue, we propose an economic NMPC formulation with a regularization on a reduced set of variables. The key idea is that we focus on a subset of states, termed critical states, and find regularization weights for these critical states only. Such an approach leads to much easier determination of regularization weights as well as less conservative performance.

3. ECONOMIC NMPC WITH REGULARIZATION OF REDUCED STATES

With a slight notational change we restate problem (1) and denote it as `eNMPC-S`:

$$\begin{aligned} & \min_{\bar{x},\hat{x},u} \psi^{ec}(x,u) \\ \text{s.t. } & \bar{x} = f_1(\bar{x},\hat{x},u) \\ & \hat{x} = f_2(\bar{x},\hat{x},u), (\bar{x},\hat{x}) \in \mathbb{X}, u \in \mathbb{U}. \end{aligned} \quad \text{(eNMPC-S)}$$

In problem `eNMPC-S`, the system states x are divided into two subsets $(\bar{x},\hat{x}) \in \mathbb{X}$. Here $\bar{x}$ represents critical states of the system, which will be regularized to stabilize the economic NMPC controller, while $\hat{x}$ represents noncritical system states. Critical states can be identified through structural analysis of the original optimization problem given by (1). For example, the states that are directly involved in the economic stage cost could be treated as critical states, since they directly affect the optimal solutions to the economic NMPC controller.

For the NMPC problem, we apply the robust problem formulation in Yang et al. (2015) by relaxing $\mathbb{X}$, written as $g(z_l) \leq 0$, with ℓ_1 penalty terms. Equivalently, we also define $g_+^{(j)}(z_l) = max(0, g^{(j)}(z_l))$, $\psi(z_l,v_l) := \psi(z_l,v_l) + \rho\|g_+(z_l)\|$, which leads to Lipschitz continuous modified stage costs needed for stability analysis. In addition,constraint qualifications and second order conditions (e.g. MFCQ, CRCQ and GSSOSC) are satisfied, and with a sufficiently large penalty weight ρ, the optimal solution of the reformulated problem is the same as the original optimization problem and the penalty terms equal zero. Similarly, terminal equality constraints can also be relaxed with ℓ_1 penalty terms. For this we choose a penalty parameter ρ_t which is large enough so that $z_N = x_s$ at the optimal solution.

We define the reformulated dynamic optimization problem for the economic NMPC controller (eNMPC) as follows:

$$\begin{aligned} V(x(k)) = \min_{\bar{z}_l,\hat{z}_l,v_l} & \sum_{l=0}^{N_1} \psi^{ec}(z_l,v_l) + \rho_t||z_N - x_s|| \\ \text{s.t.} \quad & \bar{z}_{l+1} = f_1(\bar{z}_l,\hat{z}_l,v_l) \qquad \text{(eNMPC)} \\ & \hat{z}_{l+1} = f_2(\bar{z}_l,\hat{z}_l,v_l), v_l \in \mathbb{U}, \qquad l = 0,\dots N-1. \\ & \bar{z}_0 = \bar{x}(k), \hat{z}_0 = \hat{x}(k) \end{aligned}$$

To partition the critical and noncritical system states for analysis, we introduce the following assumption.

Assumption 3. For steady state economic problem eNMPC-S, $\hat{x}$ can be uniquely determined by $(\bar{x},u)$.

Under Assumption 3, $\hat{x}$ can be uniquely calculated via the square equation system $f_2(.,.)$ with fixed values of $\bar{x}$ and u. The noncritical states $\hat{x}$ can be expressed as a function of critical states $\bar{x}$ and controls u, which leads to the steady state optimization problem:

$$\begin{aligned} & \min_{\bar{x},\hat{x},u} \psi^{ec}(x,u) \\ \text{s.t.} \quad & \bar{x} = f_1(\bar{x},\hat{x},u) \qquad \text{(eNMPC-SA)} \\ & \hat{x} = \eta(\bar{x},u), (\bar{x},\hat{x}) \in \mathbb{X}, u \in \mathbb{U}. \end{aligned}$$

While there may not be an explicit form for function $\eta(\cdot,\cdot)$, the steady state relationship exists based on implicit function theorem under Assumption 3.

Next we introduce a modified DAE system, where critical states $\bar{x}$ are determined by the original dynamic model, but noncritical states $\hat{x}$ are treated as algebraic variables. We assume that this modified system is an index 1 DAE. By defining extended states $\tilde{v}_{l+1} = v_l$, we then apply the same robust reformulation and have the following economic NMPC controller eNMPC-A:

$$\begin{aligned} V(\bar{x}(k)) = \min_{\bar{z}_l,\hat{z}_l,v_l} & \sum_{l=0}^{N-1} \psi^{ec}(z_l,v_l) + \rho_t||z_N - x_s|| \\ \text{s.t.} \quad & \bar{z}_{l+1} = f_1(\bar{z}_l,\hat{z}_l,v_l), \quad l = 0,\dots N-1 \\ & \hat{z}_l = \eta(\bar{z}_l,\tilde{v}_l), \quad l = 1,\dots N \qquad \text{(eNMPC-A)} \\ & \bar{z}_0 = \bar{x}(k) \\ & \hat{z}_0 = h(\bar{x}(k),u(k-1)), v_l,\tilde{v}_l \in \mathbb{U}. \end{aligned}$$

To simplify the regularization weight calculation and avoid over-regularization, we consider only the critical states and control variables, and add the *reduced regularization terms*, $\frac{1}{2}\|(\bar{z}_l,v_l) - (\bar{z}_s,v_s)\|^2$ to the stage costs of the unregularized controller eNMPC.

For controller eNMPC-A, where all of the noncritical states are treated as algebraic variables, a much simpler and less conservative *reduced regularization* can be obtained to guarantee its stability. Then we analyze the stability of eNMPC after adding the *reduced regularization* obtained from eNMPC-A, by considering the effect of errors introduced by this approximation. Similar to the previous analysis, we also consider a rotated stage cost defined by the steady state problem eNMPC-SA as follows:

$$\phi(x,u) = \psi^{ec}(x,u) + \lambda^T(\bar{x} - f_1(\bar{x},\eta(\bar{x},u),u) \qquad (8)$$

Note that only a subset of model equations are rotated, and λ are the multipliers for these equality constraints. Using the rotated stage cost $\phi(x,u)$ as the objective has the same solution as minimizing the original economic stage cost. Moreover, using the following parametric NLP formulation pNLP(t) with parameter t, problems eNMPC-A and eNMPC can be linked by setting $t = 0$ and $t = 1$, respectively.

$$\begin{aligned} \min_{\bar{z}_l,\hat{z}_l,v_l} & \sum_{l=0}^{N-1} \psi^{ec}(z_l,v_l) + \rho_t||z_N - x_s|| \qquad \text{(pNLP(t))} \\ \text{s.t. } & \bar{z}_{l+1} = f_1(\bar{z}_l,\hat{z}_l,v_l), l = 0,...N-1 \qquad (9) \\ & \hat{z}_l = \eta(\bar{z}_l,\tilde{v}_1) + t(f_2(\bar{z}_{l-1},\hat{z}_{l-1},v_{l-1}) - \eta(\bar{z}_l,\tilde{v}_l)), \\ & v_l,\tilde{v}_l \in \mathbb{U}, \ l = 1,\dots N \\ & \bar{z}_0 = \bar{x}(k) \\ & \hat{z}_0 = \eta(\bar{x}(k),u(k-1)) + t(\hat{x}(k) - \eta(\bar{x}(k),u(k-1))). \end{aligned}$$

Finally, for the approximation of the noncritical states, we introduce an approximation error vector $w(k) = [w_0 \dots w_N]^T$ with entries defined as follows:

$$w_0 = \hat{x}(k) - \eta(\bar{x}(k),u(k-1)) \qquad (10)$$

$$w_l = f_2(\bar{z}_{l-1},\hat{z}_{l-1},v_{l-1}) - \eta(\bar{z}_l,\tilde{v}_l) \quad l = 1\dots N \qquad (11)$$

This error vector $w(k)$ represents the differences in the values of $\hat{z}_l$ given by the dynamic function and algebraic relationship.

The following result shows that when $w(k) = 0$, the stability property can be guaranteed for controller eNMPC by adding regularization terms only for critical states $\bar{x}$ and u. In this special case, noncritical states collapse into algebraic variables and controller eNMPC is equivalent to eNMPC-A.

Theorem 4. (Proof in Yu (2017)) When $w(k) = 0$ and Assumption 3 holds, controller eNMPC can be made asymptotically stable by adding a sufficiently large regularization on v and the states $\bar{z}$.

Next we consider the stability property for controller eNMPC for cases where $w(k) \neq 0$, and the controller eNMPC can be treated as the controller eNMPC-A corrupted with non-zero $w(k)$. The process model for controller eNMPC-A is defined as follows:

$$\bar{x}(k+1) = f_1(\bar{x}(k),u(k),\eta(\bar{x}(k),u(k-1))) \qquad (12)$$

while the true process model is defined as follows:

$$\bar{x}(k+1) = f_1(\bar{x}(k),u(k),\eta(\bar{x}(k),u(k-1)) + w(k,0)) \qquad (13)$$

Here $w(k,0)$ is the first element of the error vector $w(k)$ (10), which represents the difference in the values of $\hat{x}$ at initial time for eNMPC and eNMPC-A.

To analyze the stability properties for these controllers, we consider the nominal process model (13) and model (12) for controller eNMPC-A and state the following assumptions.

Assumption 5. (Robust stability assumptions) (A) The error vector $w(k) = [w_0 \dots w_N]^T$ is drawn from a bounded set $\mathscr{W}$ with an upper bound $\bar{w}$. (B) The optimal solution to problems eNMPC and eNMPC-A is continuous with respect to $x(k)$ and w. (C) $V(x(k))$ is Lipschitz with respect to $x(k)$, with a positive Lipschitz constant L_v. (D) Model equations f_1, f_2 and steady state relationship η are Lipschitz continuous.

In particular, Assumption 5(A) is essential for our stability analysis, as it assumes bounded deviations of the dynamic noncritical states $\hat{x}$ from their algebraic approximations. For example, this occurs with noncritical states that have fast dynamics.

Along with additional standard assumptions for robust stability, we establish the ISS property for controller eNMPC-A. Moreover, because eNMPC is linked to eNMPC-A through pNLP(t), we can derive the stability property for eNMPC by treating this controller as eNMPC-A corrupted with non-zero noise terms $w(k)$. This leads to the following results.

Theorem 6. (Proof in Yu (2017)) Under Assumptions 3 and 5, controller eNMPC-A, with a sufficiently large regularization on $\bar{z}$ and v, is ISS when the process model is given by equation (13) and $w(k) \neq 0$. Moreover, under the same assumptions controller eNMPC can be made Input-to-State Practical Stable (ISpS), by adding a sufficiently large regularization on $\bar{z}$ and v.

From the above results, we can guarantee ISpS of the economic NMPC controller by only regularizing critical states $\bar{x}$, under the assumption that the deviations in noncritical states $\hat{x}$ from their algebraic predictions are bounded. In addition, if the error vector $w(k)$ is bounded by the distance of $\bar{x}$ to the optimal steady state, we can show that asymptotic stability can be established for eNMPC.

Theorem 7. (Proof in Yu (2017)) Assume for $k > K$, a finite number, $|w(k)| \leq \frac{\delta}{L_w}(|\bar{x}(k) - \bar{x}_s|)$, where $\frac{\delta}{L_w}(|\bar{x}(k) - \bar{x}_s|) \leq \bar{w}$, with $L_w = 2L_V, \delta \in [0, 1)$, then controller eNMPC can be made asymptotically stable, by adding a sufficiently large regularization on $\bar{z}$ and v.

The above properties show that, with a sufficiently large regularization on a reduced set of system states, stability of controller eNMPC can still be maintained. In this strategy, we use the process model for controller eNMPC-A to determine the reduced regularization weight. From this model we derive a reduced Hessian in the space of critical states. By making the reduced Hessian positive definite in the reduced space, we can find sufficient regularization weights for critical states. Then we add these *reduced regularization terms* to the objective of the unregularized controller eNMPC and denote this controller as eNMPC-rr. Note that we still use the original dynamic model for control, which gives accurate predictions for $\bar{x}$ and $\hat{x}$, but with a reduced regularization for the stage cost. Additional details on calculating the reduced regularization weights and stability analysis are given in Yu (2017).

Selection of critical states has a direct impact on the performance of controller eNMPC-rr. Based on the previous stability results, we observe that dynamic states that have similar performance as their algebraic counterparts are candidates for noncritical states. In particular, for states with very fast time scales, Assumption 5(A) may be satisfied implicitly and no regularization is required for these noncritical states.

4. ECONOMIC NMPC OF A SOLID SORBENT-BASED CO_2 CAPTURE SYSTEM

In previous work (Yu and Biegler (2016)), we considered a setpoint tracking case for a solid sorbent-based CO_2 capture system, where we studied setpoint tracking NMPC to control the plant and reject process disturbances. In this study we apply economic NMPC to minimize the operational cost of the CO_2 capture system, and compare the performance of various economic NMPC strategies and setpoint tracking NMPC.

The solid sorbent-based post-combustion CO_2 capture system studied in the case study is illustrated in Figure 1. In the Bubbling Fluidized Bed (BFB) adsorber, CO_2 is adsorbed via gas-solid reactions and the clean gas exists at the top. Cooling water is used to remove the reaction heat and enhance the adsorption of CO_2. The loaded solid sorbent is fed into the BFB

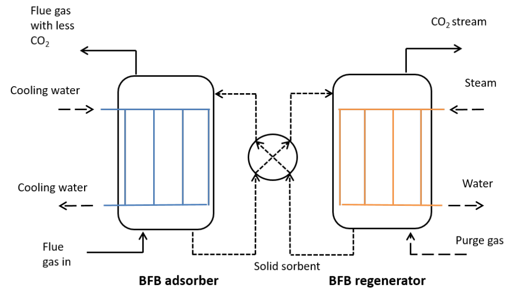


Figure 1. Schematic of the integrated carbon capture system

regenerator, which operates at higher temperature to release the CO_2 captured in the solid sorbent. In the regenerator, steam and purge gas are used to maintain high temperature, which favors the desorption process. Then fresh solid sorbent is cooled by the heat exchanger and recycled back to the adsorber. Similarly, pre-heating is also provided to loaded sorbent before it is transported into the regenerator. To model the BFB reactor, a one-dimensional, three-region, pressure driven dynamic model has been developed. Mass and heat balance equations have been written for all components in the three regions, including bubble, emulsion and cloud-wake region, which consider the effect of axial material flow and transfer terms between different regions and phases. The BFB model is open-loop stable and includes detailed transport property equations. The equation-based model and its reduction for the rigorous BFB adsorber are described in Yu et al. (2015). Here, orthogonal collocation on finite elements was applied to discretize the partial differential equations in space. Moreover, a quasi-steady state approximation replaces some of the differential states with algebraic states and a null space projection method eliminates reversible reactions for CO_2 adsorption and leads to a simplified kinetic model.

The economic NMPC problem for the integrated carbon capture system is written as problem (eNMPC). For NMPC terminal condition we use a quadratic penalty with large weights. The sampling time is 50 seconds and the prediction horizon is 1500 seconds, which is long enough to satisfy the terminal constraint implicitly. The resulting dynamic optimization problem is discretized in time using a 3-point Radau collocation on finite elements. To reduce the NLP size, we apply the input and state blocking strategy in Yu and Biegler (2016), using 5 finite elements with lengths $[50 \quad 50 \quad 200 \quad 600 \quad 600]$. The discretized model is implemented in AMPL (Fourer et al. (2002)) and the NMPC problem is solved using IPOPT (Wächter and Biegler (2006)). The simulations are conducted on an Intel i7-3770 3.40 GHz PC.

For economic NMPC problem, we minimize the operational cost of the integrated carbon capture system while satisfying the environmental constraint on the CO_2 removal fraction. The economic stage cost $\psi^{ec}(x, u) = p_1 u_1 + p_2 u_2$, where u_1 and u_2 are the manipulated variables, cooling water flowrate used to cool the fresh solid sorbent and purge gas flowrate fed into the regenerator, respectively. The corresponding unit prices are $p_1 = 10$ and $p_2 = 50$. To satisfy the environmental requirement on CO_2 capture, we add a lower bound for CO_2 removal fraction. In addition, we incorporate bounds on regenerator temperature and pressure are considered for safety reasons, and also add control input bounds and limits on maximum moves.

The steady state problem for eNMPC has over 1000 differential variables and over 7000 algebraic variables. We first determine sufficient regularization weights for all the variables using based on (7) with the strategy outlined in (Jäschke et al., 2014). However, this full regularization approach requires very large weights (up to 10^{10}) and therefore provides no performance improvement over NMPC tracking to the steady state optimum.

Next, we apply the proposed strategy to find sufficient regularization for a subset of system states. By studying the steady state optimization problem, we find that only CO_2 removal fraction is active at its lower bound for the optimal solution. Since the removal fraction is directly determined by the gas concentrations at the top of the BFB adsorber, we choose the concentrations of three gas species as critical states. In addition, we also choose a temperature state since it involves safety constraints. Besides that, we include the two manipulated variables, as they are directly involved in the economic stage cost. In the following case study, only these 6 variables make up the regularization term.

To determine sufficient regularization weights for the critical states, we calculate the reduced Hessian of the Lagrange function of (1) using numerical perturbations. The reduced Hessian is calculated at different sampling points within the feasible regions of 6 variables, and we determine the minimum regularization weights that make the reduced Hessian positive definite at all sampling points. Compared with full regularization, the calculation process is greatly simplified, since we only sample in the space of 6 variables rather than for 8000. Instead of using Gershgorin's theorem, we find the minimum regularization weight $\bar{Q} = qI$ from an eigenvalue decomposition of the reduced Hessian. For this problem the reduced Hessian matrix has small negative eigenvalues; thus we can obtain much smaller regularization weights than by using (7). From these results, we find that $q = 60$ provides a regularized reduced Hessian matrix that is positive definite at all sample points of the 6 variables.

We compare the performance of the following controllers in the case study: setpoint-tracking NMPC (`NMPC-t`), economic NMPC without regularization (`eNMPC-nr`) and economic NMPC with reduced regularization (`eNMPC-rr`). For the tracking case, the stage cost is given by quadratic tracking terms $\frac{1}{2}(\|x-x_s\|^2_{Q_x} + \|u-u_s\|^2_{Q_u})$. The weighting matrix Q_x for scaled states is an identity matrix while Q_u is a diagonal matrix with diagonal elements p_1 and p_2. For `eNMPC-nr`, only the economic stage cost $p_1u_1 + p_2u_2$ is used as objective; while for `eNMPC-rr`, a reduced regularization term $\frac{1}{2}\|(\bar{x},u)-(\bar{x}_s,u_s)\|^2_{\bar{Q}}$ with $\bar{Q} = 60I$ is added to the economic objective.

We first consider the noise-free case. Three selected state profiles and controller profiles are shown in Figure 2 and 3a. x_1 - x_3 represent the concentrations of CO_2, H_2O and N_2 at the top of BFB adsorber. From these figures we can see that all three controllers converge to the optimal steady state, including unregularized economic NMPC (`eNMPC-nr`), for which there is no stability guarantee. Here, `eNMPC-nr` penalizes the usage of u_1 and u_2 in the initial stages because the economic stage cost is directly minimized. On the other hand, this controller leads to more oscillatory control profiles than with tracking. Also, `eNMPC-rr` has a similar trend as `eNMPC-nr`, but it has smoother control profiles due to the added regularization terms.

We also compare economic performance of these controllers through the accumulated economic stage costs $\sum_{k=0}^{K}\psi^{ec}(x(k),u(k))$ during the transient process. Since the control moves become nearly steady after 20 NMPC cycles, we choose $K = 20$ and determine the cost of tracking NMPC (`eNMPC-t`) to be 4152321. Here `eNMPC-nr` achieves a 3.2% reduction in the accumulated economic stage compared to `NMPC-t`, and `eNMPC-rr` has a 2.6% improvement over `NMPC-t`, with performance sacrificed slightly due to the regularization terms.

We also consider the performance of the three controllers with additive measurement noises. In the case study, we add the noises with standard deviations of 1% of optimal steady state values. From Figure 3b, `eNMPC-nr` has the most oscillatory control profiles, especially for the purge gas fed into the regenerator. By adding the regularization terms, regularized eco-

Figure 2. Comparison of selected BFB state profiles for the noise-free case

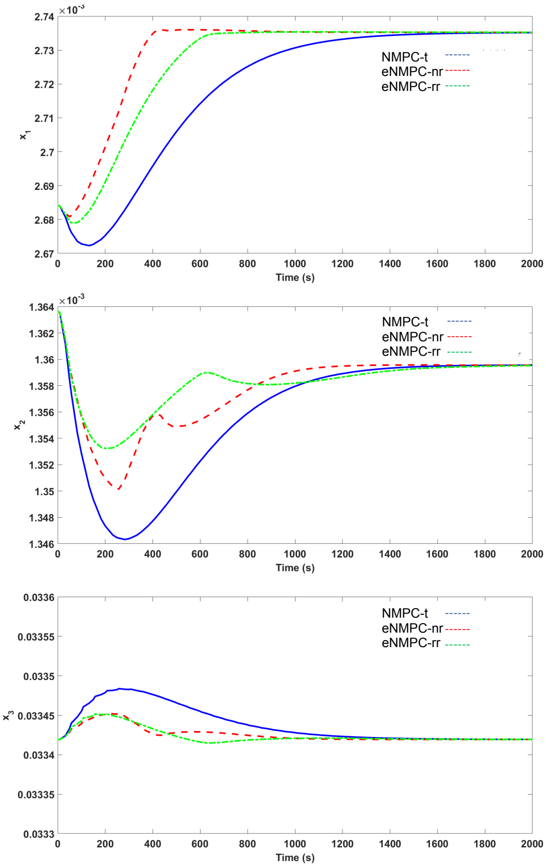
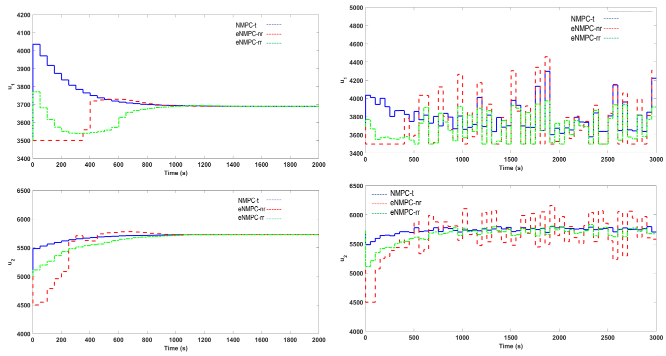


Figure 3. Comparison of BFB control profiles

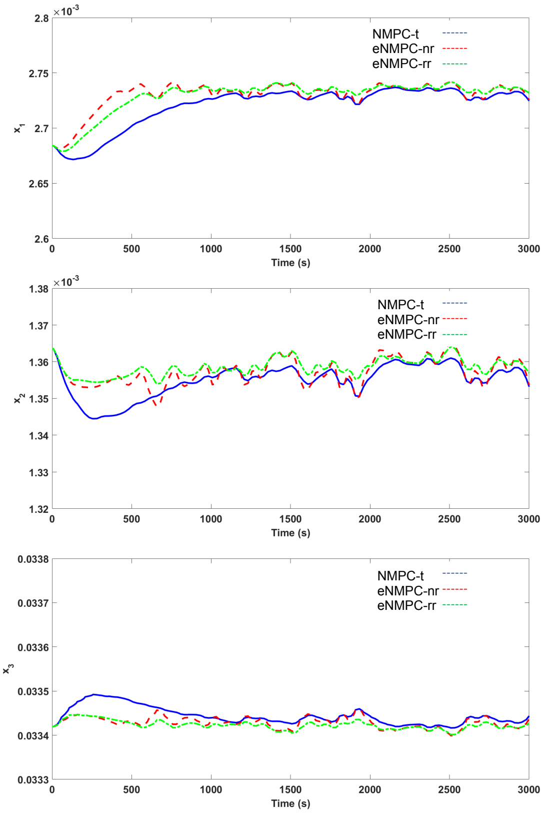


(a) Noise-free case (b) Robust case

nomic NMPC (`eNMPC-rr`) has less oscillatory control profiles and is also different from `NMPC-t`, since regularization for only 6 variables is added. From Figure 4, we can see that `eNMPC-nr` leads to the most oscillatory state profiles as well. By adding regularization terms in `eNMPC-rr`, we observe that state profiles are less oscillatory and closer to optimal steady state.

As for economic performance in the noisy case, the accumulated economic stage cost $\sum_{k=0}^{20} \psi^{ec}(x(k), u(k))$ for tracking NMPC (`NMPC-t`) is 4180054, and we observe a 3.9% improvement in economic performance with `eNMPC-nr` and a 3.1% improvement with `eNMPC-rr` over `NMPC-t`. Additional information on the performance of these controllers can be found in Yu (2017)

Figure 4. Comparison of BFB state profiles in the robust case



5. CONCLUSIONS

In this paper, we study the economic NMPC for a challenging CO_2 capture system. In general, regularization terms are needed to guarantee the stability of economic NMPC. Here we propose an economic NMPC formulation with reduced sets for regularization. Compared with full regularization, the reduced regularization strategy is much simpler to implement and leads to less conservative economic performance. To simplify the analysis, we show that algebraic variables can be removed without affecting the stability results. By applying a reduced regularization with critical states, the economic NMPC has the ISpS property, with the assumption of bounded deviations of unregulated states from their algebraic predictions. With stronger assumptions, asymptotic stability can also be achieved. The proposed strategy has been applied to an integrated CO_2 capture system, where we demonstrate that reduced regularization has desirable stability properties, while improving economic performance over setpoint tracking. In addition, determination of sufficient regularization weights for stable eNMPC is greatly simplified, especially for large-scale DAE systems.

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