Self-stabilizing Economic Nonlinear Model Predictive Control of Modular Membrane Reactor Systems

San Dinh*, Kuan-Han Lin[†], Fernando V. Lima* and Lorenz T. Biegler[†]

*Department of Chemical and Biomedical Engineering

West Virginia University, Morgantown, West Virginia 26506

Email: fernando.lima@mail.wvu.edu

[†]Department of Chemical Engineering

Carnegie Mellon University, Pittsburgh, Pennsylvania 15213

Email: lb01@andrew.cmu.edu

Abstract-In recent years, economic Nonlinear Model Predictive Control (eNMPC) has emerged as a viable alternative for distributed control systems. Because eNMPC involves the solution of a dynamic optimization problem, it provides the control actions that lead the system to the most economical transient operations, which may be periodic instead of converging to a steady state[1]. Since eNMPC has been typically used for standalone unit operations instead of plantwide control, an unsteady operation of a unit may lead to undesirable operations of downstream units. This work proposes a self-stabilizing eNMPC formulation, in which a pre-calculated steady-state condition is not required. Lyapunov functions with embedded steadystate optimal conditions are employed as additional constraints of the eNMPC formulation, so that the asymptotically stable behavior can be achieved. The performance of the proposed eNMPC is demonstrated with two case studies of a membrane reactor for natural gas utilization. In the first case study, the proposed eNMPC can effectively bring the system toward the feasible steady-state optimal operation. In the second case study, a cost-optimal steady-state does not exist due to the timevarying disturbance, and the closed-loop behavior is shown to be bounded if the disturbance is also bounded.

I. INTRODUCTION

In most industrial process control implementations, a distributed control system decouples the operation into a multilayer hierarchical architecture. The upper levels, such as the real-time optimizer and the scheduler, find the best steady-state conditions (or setpoints) with respect to an economic objective given a set of constraints (e.g., for safety, sustainability, or physical limitations), and these layers are often formulated as steady-state nonlinear programming problems. The lower levels, such as supervisory and regulatory controllers, receive the economically optimal setpoints and find a suitable sequence of dynamic control actions that steer the plant toward the desired steady-state conditions. Model Predictive Control (MPC) has been increasingly more popular for setpoint tracking at the lower level because of its ability to handle multiple-input-multiple-output dynamic systems and satisfy constraints during transient operations. Economic Nonlinear Model Predictive Control (eNMPC) is an extension of MPC that uses the nonlinear dynamic model to formulate the constraints and replaces the tracking performance objective with an economic cost objective.

When eNMPC is implemented in a stable process, the

closed-loop process can exhibit periodic behavior[1]. This is caused by the existence of a more cost-effective transient closed path around the steady-state optimal solution, and eN-MPC prioritizes the solution path with a lower operating cost. Regardless of the economic benefits, operating a process in an unsteady manner may be undesirable since it can lead to higher equipment degradation, higher operational risks, or even higher operating cost for downstream units. Thus, eNMPC is often augmented with a stabilizing constraint to drive the process toward a steady state if needed[2].

Typically, the stabilizing constraint takes the form of a Lyapunov function to guarantee asymptotic stability. To the extent of the reported literature[3], the available formulations of the Lyapunov constraints require a pre-calculated steady state, which is given by an upper layer of a distributed control system. Since the upper control layers are solved less often than the eNMPC at a regulatory control level, the provided optimal steady state might turn suboptimal when the operating conditions are shifted by the process disturbances. Motivated by this challenge, a self-stabilizing eNMPC that is independent of an external steady-state optimization is proposed in this work.

The remaining sections of this work are organized as follows. First, a review of a conventional eNMPC formulation and the basics of the Lyapunov stability theorem are provided in Section II. Then, the proposed eNMPC is formulated in Section III. Later, a case study of an implementation of the eNMPC on a modular membrane reactor is shown in Section IV. Finally, Section V presents the paper's conclusions.

II. PRELIMINARIES

A. Notation

In this work, the following notations are considered. A function $\alpha(x):\mathbb{R}_{\geq 0}\to\mathbb{R}_{\geq 0}$ is a class $\mathcal K$ function if it is continuous, strictly increasing, and $\alpha(0)=0$. A function α belongs to the class $\mathcal K_\infty$ if it belongs to the class $\mathcal K$ and is unbounded. The L^2 -norm of a vector is denoted by $\|\cdot\|$. The distance of a point $x\in\mathbb{R}^{n_x}$ from the set $A\subset\mathbb{R}^{n_x}$ is defined as $\|x\|_A:=\inf_{z\in A}\|x-z\|$. If the set $A=\{x^*\}$ only contains a single point, then $\|x\|_A:=\|x-x^*\|$ and $\lim_{x\to x^*}\|x\|_A=0$.

B. System Description

In this work, the dynamic system considered is represented by the following state-space nonlinear dynamic model:

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

$$q(x(t), u(t)) < 0 \tag{1b}$$

in which at every time instance $t, x(t) \in \mathbb{R}^{n_x}$ is the vector of states, $\dot{x}(t) \in \mathbb{R}^{n_x}$ is the vector of derivatives of the states with respect to $t, u(t) \in \mathbb{R}^{n_u}$ is the vector of manipulated variables. $f: \mathbb{R}^{n_x+n_u} \to \mathbb{R}^{n_x}$ is a set of rate of change equations that represent the process dynamics. The inequality constraints $g: \mathbb{R}^{n_x+n_u} \to \mathbb{R}^{n_g}$ represent the imposed limitations on the dynamic system, such as input and output bounds.

The following conversion is used for the time indexes:

$$t_k = k\Delta t \tag{2}$$

and the discrete-time states are defined as $x_k = x(t_k)$, the discrete-time manipulated variables are defined as $u_k = u(t_k)$ with a zero order hold. The resulting discrete-time model of (1) is:

$$x_{k+1} = \bar{f}(x_k, u_k) = x_k + \int_{t_k}^{t_{k+1}} f(x(t), u(t))$$
 (3a)

$$g(x_k, u_k) \le 0 \tag{3b}$$

in which \bar{f} is the discretization of the dynamic model (1) in time with a zero-order hold on the manipulated variables. The discretized-time difference, Δt , is assumed to be sufficiently small for the discrete-time model to accurately approximate the continuous-time model. \bar{f} is obtained by implicitly solving the continuous model (1).

C. Economic Nonlinear Model Predictive Control Formulation

At each time instance t_k , the full state information $x(t_k)$ is obtained from the measurements, and the following eNMPC subproblem is formulated as:

$$\min \quad \sum_{k=0}^{N-1} \Psi(z_k, v_k) \tag{4a}$$

s.t.
$$\overline{z_{k+1}} = \overline{f}\left(z_k, v_k\right), \quad k = 0, \dots N-1$$
 (4b)

$$z_0 = x(t_k) (4c)$$

$$q(z_k, v_k) < 0 \tag{4d}$$

in which at the predictive time step $k, z_k \in \mathbb{R}^{n_x}$ is the vector of predictive states, and $v_k \in \mathbb{R}^{n_u}$ is the vector of predictive manipulated variables. The control horizon is denoted as N, and Ψ is the stage cost that represents its operating cost.

The continuous-time dynamic model (1) is the closed form of the first-principles model since the modeling equations are directly derived from physics-based phenomena, such as equations of states or mass balances. However, in the implementation of the aforementioned eNMPC, the manipulated variables are held constant in the plant, which corresponds to a zero-order hold assumption, while the

dynamic optimization problem (4) is solved online, so a discrete-time dynamic model is more suitable for the eNMPC formulation. Additionally, the discrete-time Lyapunov-based stabilizing constraints do not require time derivatives, so they are simpler to implement than their continuous-time counterparts. For these reasons, the proposed eNMPC is formulated as a hybrid between continuous-time and discrete-time dynamics. In particular, the dynamic programming problem of the eNMPC is discretized into even partitions of the time domain, and stabilizing Lyapunov constraints are constructed from the steady-state model derived from the continuous-time dynamic model (1).

When the solution to the optimization problem (4) is available, the first stage solution of the manipulated variables, v_0 , is injected into the manipulated variables, u(t). For a closed-loop system, the eNMPC feedback control law is referred to as $u(t) = \kappa(x(t))$, and the stability analysis of the given dynamic model (1) is performed as the stability of an autonomous system of differential equations in the following subsection.

D. Asymptotically Stable Condition of Closed-Loop Systems

In this subsection, the existence of Lyapunov functions is employed to determine the asymptotic stability of a dynamic system. A brief overview of the Lyapunov stability is provided as the basis for developing the proposed stabilizing constraints in the following section.

Definition 1: A closed set A is a positive invariant set for a closed-loop system $x_{k+1} = \bar{f}(x_k, u_k) = \bar{f}(x_k, \kappa(x_k))$ if $x_k \in A$ implies $x_{k+1} \in A$.

Definition 2: A value function $V: \mathbb{R}^{n_x} \to \mathbb{R}_{\geq 0}$ is said to be a Lyapunov function for the discrete-time dynamic system $x_{k+1} = \bar{f}(x_k, \kappa(x_k))$ and a set A if \bar{f} is locally bounded, A is positive invariant, and there exist functions α_1 , α_2 of class \mathcal{K}_{∞} , and a positive definite function ϕ_d that satisfy the following:

$$\alpha_1(\|x\|_A) \le V(x) \le \alpha_2(\|x\|_A)$$
 (5)

$$V(\bar{f}(x,\kappa(x))) - V(x) \le -\phi_d(\|x\|_A) \tag{6}$$

An intuitive interpretation of the Lyapunov function, V(x), is the pseudo-potential energy of a dynamic system. The constraints in (5) force the potential energy to be zero when x is in A, and the potential energy increases indefinitely as the distance between x and set A is longer. The inequality (6) ensures that when the state x is not in the set A, the state in the following time step will approach closer to the set A. Additionally, after the states reach a point in set A, inequality (6) keeps the difference in V(x) at zero and prevents the dynamic process from moving out of the positive invariant set A. Thus, the existence of a Lyapunov function implies the asymptotic convergence to a set A. Lyapunov stability is indicated by the following well-known theorem[4]:

Theorem 1: Given a positive invariant set A for $x_{k+1} = \bar{f}(x_k, \kappa(x_k))$ and a locally bounded function \bar{f} , if a Lyapunov function V for \bar{f} and the set A exist, then the dynamic system asymptotically converges to a stable steady state in A.

III. SELF-STABILIZING ECONOMIC MODEL PREDICTIVE CONTROL FORMULATION

A. Steady-state Optimal Conditions

The steady-state optimization is formulated by combining the steady-state model derived from the dynamic model (1) and the economic objective of the eNMPC in (11a). Formally, it is defined as below:

$$(x^*,u^*) := \underset{x,u}{\operatorname{argmin}} \quad \Psi\left(x,u\right) \tag{7a}$$
 s.t.
$$f(x,u) = 0 \tag{7b}$$

s.t.
$$f(x, u) = 0$$
 (7b)

$$g(x, u) \le 0 \tag{7c}$$

in which x^* and u^* are respectively the optimal steady-state solutions of the states and manipulated variables, f and qare respectively the rates of change and the model constraints given in (1). An equivalent steady-state optimization problem is formulated by translating the inequality constraints to barrier terms in the objective function:

$$\min_{x,u} \phi(x,u) := \Psi(x,u) + \mu \sum_{j=1}^{n_g} \ln(-g_j(x,u))$$
 (8a)

$$s.t. f(x,u) = 0 (8b)$$

in which $\mu > 0$ is the barrier parameter, and n_g is the number of inequality constraints. The KKT conditions for the reformulated steady-state optimization in (8) are given as follows:

$$-\nabla_{u} f(x, u) \left(\nabla_{x} f(x, u)\right)^{-1} \nabla_{x} \phi(x, u) + \nabla_{u} \phi(x, u) = 0$$
(9a)

$$f(x,u) = 0 (9b)$$

In addition to the KKT conditions, the second-order sufficient conditions for optimality are assumed to always hold. Additionally, the matrix $\nabla_x f$ is assumed to always be nonsingular, and the linear independence constraint qualification is satisfied.

For ease of notation in the following subsections, the left-hand side of the equation (9a) is referred to as the reduced gradient that is denoted as $Z(x,u)^{\top} \nabla \phi(x,u)$ with $Z(x,u)^{\top} = \left[-\nabla_u f(x,u) \left(\nabla_x f(x,u) \right)^{-1} \right] I.$

In the above KKT conditions, the matrix inverse of the term $(\nabla_x f(x,u))^{-1}$ can be performed by a symbolic toolbox. However, the explicit form is difficult to compute for a large-scale dynamic system. To address this challenge, the KKT constraint (9a) can be replaced by (10), where the quantity \mathcal{M} is defined in (10b) so that (10a) is equivalent

$$Z(x,u)^{\top} \nabla \phi(x,u) = -\nabla_u f(x,u) \mathcal{M} + \nabla_u \phi(x,u)$$

$$= 0$$

$$\nabla_x \phi(x,u) = (\nabla_x f(x,u)) \mathcal{M}$$
(10a)
(10b)

$$\nabla_x \phi(x, u) = (\nabla_x f(x, u)) \mathcal{M}$$
 (10b)

B. Self-stabilizing Lyapunov Constraints

Conventionally, the distance from an asymptotically stable set, $||x||_A$, is defined as the L^2 -norm of the difference, $||x-x^*||$, from a steady-state optimal solution, x^* , of (7).

However, this implies that (7) is required to be solved before solving the optimization of the eNMPC. To avoid solving two separate optimization problems, the optimality conditions of (7) are derived and used for the formulation of the additional stabilizing constraint of the eNMPC.

From the definitions and properties of the Lyapunov functions, the following modification of the eNMPC is proposed for the self-stabilizing eNMPC:

min
$$\sum_{k=0}^{N-1} \Psi(z_k, v_k) + \beta \Phi(z_{N-1}, z_N, v_{N-1})$$
 (11a)

s.t.
$$z_{k+1} = \bar{f}(z_k, v_k), \quad k = 0, \dots N - 1$$
 (11b)

$$z_0 = x(t_k) \tag{11c}$$

$$V(x_k) - V(x_{k-1}) \le -\delta \phi_d(x_{k-1}), \delta \in (0, 1]$$
 (11d)

$$g(z_k, v_k) \le 0 \tag{11e}$$

in which the parameter δ determines the speed of convergence to the steady-state optimal point, and Φ is the additional terminal cost. Also, β is a sufficiently large weighting of the terminal cost to ensure asymptotic stability of an eNMPC with short horizon N.

Since an eNMPC with Lyapunov stabilizing constraint is formulated to maintain the process at the most economic steady state, x^* , with respect to an objective function in the form of (11a), a set A of all achievable steady-state economically optimized states is positive invariant.

The terminal cost Φ , the Lyapunov function V and the Lyapunov stage cost ϕ_d in (11d) are chosen as below:

$$\Phi(z_{N-1}, z_N, v_{N-1}) := \|(z_N - z_{N-1})\|^2 + \|Z(z_N, v_{N-1})^\top \nabla \phi(z_N, v_{N-1})\|^2$$
(12)

$$\phi_d(x_{k-1}) := ||x_k - x_{k-1}||^2 + ||Z(x_{k-1}, u_{k-1})^\top \nabla \phi(x_{k-1}, u_{k-1})||^2$$
(13)

$$V(x_k) := \sum_{l=0}^{N-1} (\phi_d(z_l)) + \Phi(z_{N-1}, z_N, v_{N-1})$$
 (14)

At a fixed discrete-time instance k, the state vector x_k is given by the measurements, the previous state vector, x_{k-1} , and previous manipulated variables, u_{k-1} , which are available from the process data historian. Thus, the preceding time $\phi_d(x_{k-1})$ is constant at time k. In equation (14), the Lyapunov function is defined with respect to the prediction of the eNMPC. Therefore, at time k, the term $V(x_{k-1})$ in the constraint (11d) is determined by the solution of the eNMPC in the previous time step and has a constant value. As a result, the only term in (11d) that contains independent variables of the dynamic optimization (11) is $V(x_k)$, and the remaining terms of (11d) are updated after a new solution of the eNMPC is achieved.

In equations (12) to (13), the self-stabilizing eNMPC replaces the $||x-x^*||$ of the conventional eNMPC with the square of the deviation from the KKT conditions given in (9). Additionally, $V(x_k)$ approaches zero as x_k approaches x^* , so the process is moved toward the steady-state optimal solution without knowing the pre-computed value of x^* . Moreover, the asymptotic stability is proven as below.

By definition, $V(x_k)$ is a sum of squares, so it is positive definite. The following inequality and equation are true for any feasible states:

$$V(x_0) \ge V(x_0) - V(x_{M+1}) \tag{15}$$

$$V(x_0) - V(x_{M+1}) = \sum_{k=0}^{M} (V(x_k) - V(x_{k+1}))$$
 (16)

By combining (15) and (16), and letting M approach ∞ , the manipulation gives:

$$V(x_0) \ge \sum_{k=0}^{\infty} (V(x_k) - V(x_{k+1}))$$
 (17)

The inequality (17) and the constraint (11d) lead to the following inequality:

$$V(x_0) \ge \sum_{k=0}^{\infty} \delta \phi_d(x_k) \tag{18}$$

The right-hand side of the inequality (18) is a monotonically non-decreasing function that is bounded above, which implies that:

$$\lim_{k \to \infty} \phi_d(x_k)$$
= $\|x_{k+1} - x_k\|^2 + \|Z(x_k, u_k)^T \nabla \phi(x_k, u_k)\|^2$ (19)
= 0

Therefore, the closed-loop process with the self-stabilizing eNMPC asymptotically approaches the steady-state optimal condition of (7), as long as the system described by (1) has a steady state. In the next section, we will demonstrate this property and consider input disturbances for which the cost-optimal steady state does not exist.

IV. APPLICATION TO MODULAR MEMBRANE REACTOR

In this section, the proposed eNMPC formulation is demonstrated via an application to a cocurrent membrane reactor for direct methane aromatization (DMA-MR). The schematic of the considered DMA-MR is shown in Figure 1. The main function of this membrane reactor is to convert methane from natural gas feed to benzene and hydrogen[5].

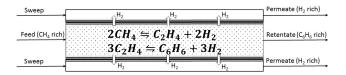


Fig. 1: Schematic of DMA-MR with inputs, outputs, and reactions

In the shell-and-tube DMA-MR, the reactions take place in the tube, and the membrane layer, which is placed on the surface of the tube wall, is highly selective toward hydrogen permeation. The reaction equilibrium shifts toward the products when hydrogen is removed from the reactive tube, which leads to higher methane conversion when compared to a stand-alone reactor system.

The detailed dynamic model of the DMA-MR is provided in the reference[6], and the DMA-MR is controlled by manipulating the tube flow rate and the shell flow rate. It is assumed that the dynamic model also has temperature and pressure controlled, so the DMA-MR is considered to be isothermal and isobaric. Flow rates are presumed to be driven by pressure profiles in the tube and shell, and pressure drops are negligible. The DMA-MR is assumed to have radial and angular symmetry, and it is considered only to change states along its length. The resulting dynamic model of the DMA-MR is a system of partial differential equations with differential independent variables as the operational time and the length of the DMA-MR. The method of lines is applied to discretize the DMA-MR length into equal differential length partitions in order to solve this model. Consequently, the dynamic model of the DMA-MR can be defined as a nonlinear state-space model of the system of ordinary differential equations that represents a system of nonlinear state-space dynamics.

Due to the nature of the dynamic model being a first-principles model, only the continuous-time formulation of the model is explicitly available, and the discrete-time dynamic model has to be implicitly solved with the eNMPC dynamic programming problem. In such situations, the proposed continuous-discrete hybrid formulation of the self-stabilizing eNMPC is directly applicable to any modeling language that has fixed-time step discretization. In this work, the Pyomo modeling tool[7] is used to construct the dynamic model, and the dynamic optimization problem of the controller is solved with the Ipopt solver[8].

The economic stage cost for the eNMPC implementation of the DMA-MR is based on the price of the products (benzene and hydrogen) and the separation cost of the permeate and the retentate streams, which are assumed to be proportional to the respective flow rates. Formally, the economic stage cost at time k, Ψ_k , is defined as the following:

$$\Psi_k = -(30C_{C_6H_6,k} - 0.5) Q_{tube,k} -(2C_{H_2,k} - 0.5) Q_{shell,k}$$
(20)

in which at a fixed discrete-time value k, $Q_{tube,k}$ is the tube flow rate, $Q_{shell,k}$ is the shell flow rate, $C_{C_6H_6,k}$ is the concentration of benzene in the retentate, and $C_{H_2,k}$ is the concentration of hydrogen in the permeate. In this case study, the weights of benzene, hydrogen, and separation cost in (20) do not reflect the actual monetary values for a techno-economic analysis. Instead, they suggest the relative differences between the prices of all elements in the economic objective. Thus, Ψ_k and the subsequently defined average profit in (21), \bar{P} , have the unit in the domain of currency over time, and their numerical values are best used for comparisons between different eNMPC formulations.

In the first case study, the proposed self-stabilizing eN-MPC in (11) and the conventional eNMPC (4) are implemented as feedback controllers for the DMA-MR, and their performances are compared to demonstrate the advantage of the proposed framework. Both eNMPC formulations have the predictive horizon of 10 minutes, which is discretized with even time differences of 1 minute into 10 predictive time steps. Their closed-loop simulations are initialized at a suboptimal steady state with a tube flow rate of 700 $dm^3/minute$ and a shell flow rate of 15000 $dm^3/minute$. The weighting parameter, β , of the terminal cost of the self-stabilizing eNMPC is chosen to be 10^5 , and the Lyapunov parameter, δ , is chosen to be 0.1 for all of the following simulations.

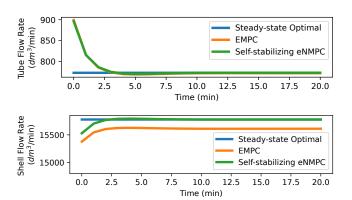


Fig. 2: Comparison of the manipulated variable profiles of the DMA-MR under different closed-loop eNMPC formulations

The resulting solutions of the manipulated variables under the different eNMPC feedback laws are depicted in Figure 2, and the closed-loop product concentration of the outlets of the DMA-MR are illustrated in Figure 3. Since the predictive horizon of both eNMPC formulations is intentionally chosen to be insufficiently short, the conventional eNMPC fails to reach the steady-state optimum. However, the sufficiently large terminal cost of the self-stabilizing eNMPC is able to bring the DMA-MR to the steady-state optimum without separately solving the steady-state optimization to obtain a pre-calculated setpoint for the terminal cost.

The average profit, \bar{P} , of each closed-loop profile is the negative of the mean of the average stage cost Ψ_k for all k in the simulated horizon, N_{sim} . Mathematically, \bar{P} is defined as:

$$\bar{P} = \frac{-1}{N_{\text{sim}}} \sum_{k=0}^{N_{\text{sim}}} \Psi_k$$
 (21)

From the simulation results, the average profit of the conventional eNMPC is 3.55, while the average profit of the self-stabilizing eNMPC is 3.59. In the case of the DMA-MR, the average profit is highest at an optimal steady-state operation instead of a periodic operation, so an eNMPC that brings the system closer to the steady-state optimal solution has a higher average profit. It is important to note that the main driving force of the system to the cost-optimal steady

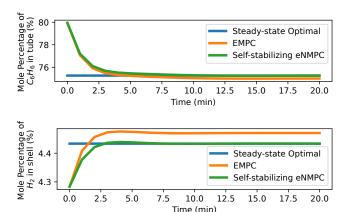


Fig. 3: Comparison of the output variable profiles of the DMA-MR under different closed-loop eNMPC formulations

state is the terminal cost in (12), and the Lyapunov constraint (11d) is not active during the transient process to reach a new steady state. The main function of the Lyapunov constraint here is to promote convergence to a steady state if the closed-loop process is otherwise not asymptotically stable. On the other hand, the closed-loop system of the DMA-MR with a terminal penalty appears to be asymptotically stable, so an active Lyapunov constraint holds but may remain inactive when reaching a new steady state. To prevent the Lyapunov constraints from forcing the system to rapidly approach the cost-optimal steady state, the Lyapunov parameter, δ , is chosen to be small in this case study, which results in a more cost-effective transient operation.

In the second case study, dynamic disturbances are considered to further understand the specific stabilizing features of the proposed eNMPC. An important note on the selfstabilizing eNMPC is that the constraint (11d) only stabilizes the self-imposed fluctuations by the closed-loop eNMPC. When the process is under the effect of external disturbances, the self-stabilizing eNMPC by itself is unable to bring the process to a steady state. To illustrate the disturbance effects on the self-stabilizing eNMPC, a sinusoidal wave is added to the inlet concentration of methane to mimic changes in the process feed coming from an upstream process. Two self-stabilizing eNMPC formulations are considered for the disturbance effect analysis. The first self-stabilizing eNMPC is a feedback controller that only updates the value of the disturbance in the dynamic programming problem after a new state information is available. The second self-stabilizing eNMPC is a feedforward controller with an accurate disturbance predictive model augmented to the dynamic model.

Both eNMPC formulations have the same tuning of the Lyapunov parameters $\delta=1$, and the prediction horizons are set to $10\ minutes$, which is discretized with even time differences of $1\ minute$ into $10\ predictive$ time steps. The simulations of the closed-loop system with different eNMPC formulations are initialized at the same steady state, that is the steady-state solution of the DMA-MR with the inlet tube flow rate of $800\ dm^3/min$ and the inlet shell flow rate of

9000 dm^3/min .

The resulting solutions of the manipulated variables of both feedback and feedforward eNMPC formulations are shown in Figure 4, and the closed-loop product concentration of the outlets of the DMA-MR are illustrated in Figure 5. Since the feedforward eNMPC receives the information on the disturbance ahead of time, the controller adjusts the manipulated variables to compensate for the effects before the disturbance further upsets the system. The feedback eNMPC only receives the disturbance information after the DMA-MR system is already affected. For this reason, while both feedback and feedforward eNMPC follow a similar trend, the trend of the feedforward eNMPC is one time-step ahead of the trend of the feedback eNMPC, and this behavior can be observed in Figures 4 and 5.

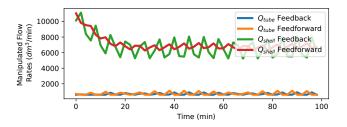


Fig. 4: Feedback and feedforward manipulated variables of self-stabilizing eNMPC under disturbances

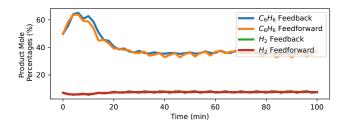


Fig. 5: Feedback and feedforward output variables of self-stabilizing eNMPC under disturbances

From the simulation results, the average profit of the feedback eNMPC is 1.27, and the average profit of the feedforward eNMPC is 1.41. In the case of the DMA-MR, the average profit is highest at an optimal steady-state operation instead of a periodic operation, so an eNMPC that brings the system closer to the steady-state optimum has a higher average profit. Thus, for DMA-MR with disturbance scenarios, feedforward eNMPC is more cost-effective than the feedback eNMPC.

For the disturbance effect case study, the Lyapunov parameter ($\delta=1$) is chosen at a significantly higher value when compared to the previous case study. As a result, the Lyapunov constraint (11d) is sometimes active in the simulations. However, as shown in Figures 4 and 5, sinusoidal disturbances do not lead to a steady state for the dynamic system, and asymptotic stability does not hold, as the optimal solution is constantly changing at every time step. Because

the Lyapunov constraint follows this time-varying steadystate optimal solution, the closed-loop behavior is bounded according to the disturbance realization.

V. CONCLUSIONS

In this work, a self-stabilizing eNMPC is proposed to prevent the self-imposed unsteady operation of a closed-loop system. The proposed eNMPC can be independently implemented without a pre-calculated steady-state condition for the Lyapunov stabilizing constraint. By reformulating the Lyapunov functions using the KKT conditions of the respective steady-state economic optimization, the closed-loop asymptotic stability is achieved at the steady-state optimal solution.

An eNMPC framework for the modular DMA-MR is proposed using the self-stabilizing eNMPC, and the framework is demonstrated to be an effective control system for nonlinear dynamic systems that admit steady states. In the first case study, the proposed eNMPC is able to reach the cost-optimal steady state, so it outperforms the conventional eNMPC without a pre-calculated steady-state optimum. In the second case study, a cost-optimal steady state does not exist in the presence of bounded time-varying disturbances. Nevertheless, the closed-loop behavior of the proposed eNMPC is still bounded instead of becoming unstable. The robust behavior for eNMPC will be analyzed further in future work.

ACKNOWLEDGMENTS

The authors thank the National Science Foundation for providing the funding support via the CAREER Award 1653098, and the Center for Advanced Process Decision-making at Carnegie Mellon University for providing the additional funding support for this research.

REFERENCES

- [1] D. Angeli, R. Amrit, and J. B. Rawlings, "On Average Performance and Stability of Economic Model Predictive Control," *IEEE Trans. Automat. Contr.*, vol. 57, no. 7, pp. 1615–1626, July 2012.
- [2] D. W. Griffith, V. M. Zavala, and L. T. Biegler, "Robustly Stable Economic Nmpc for Non-Dissipative Stage Costs," *Journal of Process Control*, vol. 57, pp. 116–126, 2017.
- [3] J. B. Rawlings, D. Angeli, and C. N. Bates, "Fundamentals of economic model predictive control," in 2012 IEEE 51st IEEE Conference on Decision and Control (CDC). Maui, HI, USA: IEEE, Dec. 2012, pp. 3851–3861.
- [4] J. B. Rawlings and D. Q. Mayne, Model Predictive Control: Theory and Design. Madison, Wis: Nob Hill Pub, 2009.
- [5] J. C. Carrasco and F. V. Lima, "An Optimization-Based Operability Framework for Process Design and Intensification of Modular Natural Gas Utilization Systems," *Computers & Chemical Engineering*, vol. 105, pp. 246–258, Oct. 2017.
- [6] S. Dinh and F. V. Lima, "Dynamic Operability Analysis for Process Design and Control of Modular Natural Gas Utilization Systems," *Ind. Eng. Chem. Res.*, vol. 62, no. 5, pp. 2052–2066, Feb. 2023.
- [7] W. E. Hart, C. D. Laird, J.-P. Watson, D. L. Woodruff, G. A. Hackebeil, B. L. Nicholson, and J. D. Siirola, *Pyomo — Optimization Modeling in Python*, ser. Springer Optimization and Its Applications. Cham: Springer International Publishing, 2017, vol. 67.
- [8] A. Wächter and L. T. Biegler, "On the Implementation of an Interior-Point Filter Line-Search Algorithm for Large-Scale Nonlinear Programming," *Math. Program.*, vol. 106, no. 1, pp. 25–57, Mar. 2006.