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# Safe economic model predictive control of nonlinear systems\*

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# ABSTRACT

This work focuses on the design of a new class of economic model predictive control (EMPC) systems for nonlinear systems that address simultaneously the tasks of economic optimality, safety and closed-loop stability. This is accomplished by incorporating in the EMPC an economics-based cost function and Control Lyapunov-Barrier Function (CLBF)-based constraints that ensure that the closed-loop state does not enter unsafe sets and remains within a well-characterized set in the system state-space. The new class of CLBF-EMPC systems is demonstrated using a nonlinear chemical process example.

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#### 1. Introduction

Since operational efficiency and increasing energy consumption are becoming crucially important issues in the chemical and petrochemical industry, a model-based feedback control strategy, economic model predictive control (EMPC), has been proposed as an efficient method to address process control problems integrated with dynamic economic optimization of the process (e.g., [1–4]). EMPC allows the chemical process to be operated in a time-varying fashion (off steady-state) to dynamically optimize process economic performance, and incorporates constraints that guarantee closed-loop stability and feasibility within an explicitly-defined estimate of the closed-loop stability region under an appropriate control law (e.g., a Lyapunov-based feedback control law).

On the other hand, process operational safety is of significant importance in the chemical process industries due to the disastrous consequences unsafe operation has for both lives and property [5,6]. Despite the widely-used safety protection instruments applied in industry (e.g., alarm systems, emergency shut-down systems, and safety relief devices), the potential for unsafe process operation caused by multi-variable interactions motivates the development of improved process design and process operational safety methods. Several recent works have proposed a method that

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combines control and safety within a systems framework using a function termed the Safeness Index that indicates the relative safeness of the process states (e.g., [7]). It has been shown that under the EMPC integrated with Safeness Index function-based constraints, closed-loop stability and operational safety of nonlinear chemical process systems can be achieved. At this stage, however, the problem of incorporating safety region constraints in EMPC to deal with process operational safety and ensuring the feasibility of the resulting EMPC a priori has not been studied.

Recently, a control method termed Control Lyapunov-Barrier Function (CLBF)-based control (e.g., [8,9]) has been proposed for the control system design that accounts for both closed-loop stability and safety. Typically, CLBFs can be formulated through the weighted average of a Control Lyapunov Function (CLF) and a Control Barrier Function (CBF), and therefore they possess similar stabilizability and safety properties to those associated with the CLF and CBF from which they can be derived. In a recent work [10], a CLBF was combined with tracking MPC to drive the state of a closed-loop nonlinear system to its set point while avoiding the unsafe region in state-space. At this stage, however, it remains an open issue to incorporate a CLBF into EMPC design to obtain closedloop stability, process operational safety, and optimal economic benefits simultaneously.

These safety and stability considerations motivate the development of CLBF-based EMPC that integrates a Control Lyapunov-Barrier Function with EMPC to account for input constraints, safety considerations, and the stability of the closed-loop system. The proposed methodology is applied to a nonlinear chemical process example to demonstrate the ability of the CLBF-EMPC to operate the process in an economically optimal manner while avoiding an unsafe region in the state-space.

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## 2. Preliminaries

#### 2.1. Notation

The notation  $|\cdot|$  is used to denote the Euclidean norm of a vector.  $x^T$  denotes the transpose of x. The notation  $L_f V(x)$  denotes the standard Lie derivative  $L_f V(x) := \frac{\partial V(x)}{\partial x} f(x)$ . Set subtraction is denoted by "\", i.e.,  $A \setminus B := \{x \in \mathbb{R}^n \mid x \in A, x \notin B\}$ . Ø signifies the null set. Given a set  $\mathcal{D} \subset \mathbb{R}^n$ , we denote the boundary of  $\mathcal{D}$  by  $\partial \mathcal{D}$ , and the closure of  $\mathcal{D}$  by  $\overline{\mathcal{D}}$ .  $\mathcal{B}_{\beta}(\epsilon) := \{x \in \mathbb{R}^n \mid |x-\epsilon| < \beta\}$  is an open ball around  $\epsilon$  with radius of  $\beta$ . The function  $f(\cdot)$  is of class  $\mathcal{C}^1$  if it is continuously differentiable in its domain. A continuous function  $\alpha : [0, \alpha) \rightarrow [0, \infty)$  is a class  $\mathcal{K}$  function if it is strictly increasing and is zero only when evaluated at zero. A scalar function  $V : \mathbb{R}^n \rightarrow \mathbb{R}$  is proper if the set  $\{x \in \mathbb{R}^n \mid V(x) \le k\}$  is compact  $\forall k \in \mathbb{R}$ , or equivalently, V is radially unbounded [11].

#### 2.2. Class of systems

The class of continuous-time nonlinear systems considered is described by the following system of first-order nonlinear ordinary differential equations:

$$\dot{x} = f(x) + g(x)u + h(x)w, \ x(t_0) = x_0 \tag{1}$$

where  $x \in \mathbf{R}^n$  is the state vector,  $u \in \mathbf{R}^m$  is the manipulated input vector, and  $w \in W$  is the disturbance vector, where  $W := \{w \in \mathbf{R}^q \mid |w| \le \theta, \theta \ge 0\}$ . The control action constraint is defined by  $u \in U := \{u_i^{\min} \le u_i \le u_i^{\max}, i = 1, ..., m\}$ .  $f(\cdot)$ ,  $g(\cdot)$ , and  $h(\cdot)$ are sufficiently smooth vector and matrix functions of dimensions  $n \times 1$ ,  $n \times m$ , and  $n \times q$ , respectively. Throughout the manuscript, the initial time  $t_0$  is taken to be zero ( $t_0 = 0$ ), and it is assumed that f(0) = 0, and thus, the origin is a steady-state of the nominal (i.e.,  $w(t) \equiv 0$ ) system of Eq. (1) (i.e.,  $(x_s^*, u_s^*) = (0, 0)$ , where  $x_s^*$  and  $u_s^*$  represent the steady-state state and input vectors, respectively).

#### 2.3. Control Lyapunov-Barrier Function (CLBF)

In this work, we develop an economic model predictive control design that utilizes a Control Lyapunov-Barrier Function [12] in designing the constraints to maintain the closed-loop state in a safe operating region at all times in the following sense:

**Definition 1.** Consider the system of Eq. (1) with input constraints  $u \in U$ , and an open set  $\mathcal{D}$  in state-space within which it is unsafe for the system to be operated. If there exists a control law  $u \in U$  such that the state trajectories of the system for any initial state  $x(0) = x_0 \in \mathcal{U} \subset \mathbb{R}^n$  satisfy  $x(t) \in \mathcal{U}, \forall t \ge 0$ , where  $\mathcal{U} \cap \mathcal{D} = \emptyset$ , we say that process operational safety is achieved in the sense that the control law u maintains the process state within a safe operating region  $\mathcal{U}$  at all times.

Based on the original Control Lyapunov-Barrier Function (CLBF) [12] that was developed for the nominal system of Eq. (1) with  $w(t) \equiv 0$ , in this manuscript, we propose a constrained CLBF that accounts for the input constraints  $u \in U$  in the system of Eq. (1), and is stabilizing even in the presence of small bounded disturbances w(t). Specifically, the definition of a constrained CLBF is as follows:

**Definition 2.** Given a set of unsafe points in state-space  $\mathcal{D}$  (i.e., the unsafe region), a proper, lower-bounded and  $\mathcal{C}^1$  function  $W_c(x)$ :  $\mathbb{R}^n \to \mathbb{R}$  is a constrained CLBF if it has a minimum at the origin and

satisfies the following properties:

$$W_{c}(x) > \rho_{c}, \quad \forall x \in \mathcal{D} \subset \phi_{uc}$$

$$L_{f}W_{c}(x) < 0,$$
(2a)

$$\forall x \in \{z \in \phi_{uc} \setminus (\mathcal{D} \cup \{0\} \cup \mathcal{X}_e) \mid L_g W_c(z) = 0\}$$
(2b)

$$\mathcal{U}_{\rho_c} := \{ x \in \phi_{uc} \mid W_c(x) \le \rho_c \} \neq \emptyset$$
(2c)

$$\overline{\phi_{uc} \setminus (\mathcal{D} \cup \mathcal{U}_{\rho_c})} \cap \overline{\mathcal{D}} = \emptyset \tag{2d}$$

where  $\rho_c \in \mathbf{R}$  and  $\mathcal{X}_e := \{x \in \phi_{uc} \setminus (\mathcal{D} \cup \{0\}) \mid \partial W_c(x)/\partial x = 0\}$ is a set of states where  $L_f W_c(x) = 0$  due to  $\partial W_c(x)/\partial x = 0$ .  $\phi_{uc}$  is defined to be the union of the origin,  $\mathcal{X}_e$  and the set where the timederivative of  $W_c(x)$  is negative with constrained input:  $\phi_{uc} = \{x \in \mathbf{R}^n \mid \dot{W}_c(x(t), u(t)) = L_f W_c + L_g W_c u < 0, u = \Phi(x) \in U\} \cup \{0\} \cup \mathcal{X}_e$ .  $\Phi(x)$  is a nonlinear feedback control law, which will be discussed in detail in the next subsection.

#### 2.4. Stabilization and safety via CLBF

We assume that there exists a feedback control law  $u = \Phi(x) \in U$  (e.g., the universal Sontag control law [13]) such that the state of the closed-loop nominal system of Eq. (1) is bounded in a level set of  $W_c(x)$  embedded in an open neighborhood D that includes the origin in its interior in the sense that there exists a  $C^1$  constrained Control Lyapunov-Barrier function  $W_c(x)$  that has a minimum at the origin and where the following inequalities hold for all  $x \in D$ :

$$\alpha_1(|x|) \le W_c(x) - \rho_0 \le \alpha_2(|x|), \tag{3a}$$

$$\frac{\partial W_c(x)}{\partial x} F(x, \Phi(x), 0) \le 0, \tag{3b}$$

$$\left|\frac{\partial W_c(x)}{\partial x}\right| \le \alpha_4(|x|) \tag{3c}$$

where  $\alpha_j(\cdot), j = 1, 2, 4$  are class  $\mathcal{K}$  functions, and  $W_c(0) = \rho_0$  is the global minimum value of  $W_c(x)$  in D. F(x, u, w) is used to represent the system of Eq. (1) (i.e., F(x, u, w) = f(x) + g(x)u + h(x)w). By continuity and the smoothness assumed for f, g and h, there exists a positive constant M such that  $|F(x, u, w)| \leq M$  holds for all  $x \in \mathcal{U}_{\rho_c}, u \in U$  and  $w \in W$ . Also, there exist positive constants  $L_x, L_w, L'_x$  such that the following inequalities hold for all  $x, x' \in \mathcal{U}_{\rho_c}, u \in U$  and  $w \in W$ :

$$|F(x, u, w) - F(x', u, 0)| \le L_x |x - x'| + L_w |w|$$

$$|\partial W_x(x) = |A| = |A|$$

$$\frac{\partial W_{\ell}(x)}{\partial x}F(x, u, w) - \frac{\partial W_{\ell}(x)}{\partial x}F(x', u, 0)\Big| \leq L'_{x}|x - x'| + L'_{w}|w|$$
(4b)

The following theorem provides sufficient conditions under which the existence of a constrained CLBF of Eq. (2) for the system of Eq. (1) under the control law  $u = \Phi(x) \in U$  guarantees that the solution of the system of Eq. (1) always stays in a safe operating region.

**Theorem 1.** Consider that a constrained CLBF  $W_c(x) : \mathbf{R}^n \to \mathbf{R}$  that has a minimum at the origin and meets the conditions of Eq. (2), exists for the nominal system of Eq. (1) with  $w(t) \equiv 0$  subject to input constraints, defined with respect to a set of unsafe points  $\mathcal{D}$  in statespace. The feedback control law  $u = \Phi(x) \in U$  guarantees that the closed-loop state stays in  $\mathcal{U}_{\rho_c}$  for all times for  $x(0) = x_0 \in \mathcal{U}_{\rho_c}$ , and does not enter  $\mathcal{D}$  for  $x_0 \in \phi_{uc} \setminus \mathcal{D}$ .

**Proof.** We first prove that if  $x_0 \in U_{\rho_c}$ , the closed-loop state x(t) is always bounded in  $U_{\rho_c}$  and never enters  $\mathcal{D}$ , for all  $t \ge 0$ . Based on the definition of  $\phi_{uc}$ , it is trivial to show that  $\dot{W}_c$  remains negative within the set  $U_{\rho_c} \setminus (X_e \cup \{0\})$  using the controller  $u = \Phi(x) \in U$ .

It follows that  $W_c(x(t)) < W_c(x_0)$  for all  $x_0 \in \mathcal{U}_{\rho_c} \setminus \{\mathcal{X}_e \cup \{0\}\}$ . Additionally, since there exists the set of states  $x_e \in \mathcal{X}_e$  where  $\partial W_c(x)/\partial x = 0$ , the closed-loop state may converge to  $x_e$  instead of the origin under  $u = \Phi(x)$  (e.g.,  $x_e$  is a saddle point or a local minimum on  $\mathbb{R}^n$ ). Therefore, the state is always bounded in the set  $\mathcal{U}_{\rho_c}$ . Additionally, since  $W_c$  is a proper function and  $\dot{W}_c \leq 0$  holds under the controller  $\Phi(x)$ , it follows that the level set  $\mathcal{U}_{\rho_c}$  of  $W_c(x)$  is a compact invariant set, which is a nice property similar to properties which can be obtained from a Lyapunov function. Due to the fact that  $\mathcal{U}_{\rho_c} \cap \mathcal{D} = \emptyset$ , it is apparent that for all  $x_0 \in \mathcal{U}_{\rho_c}$ , the closed-loop state x(t),  $\forall t > 0$  does not enter the unsafe region  $\mathcal{D}$  any time. Since any subset of  $\mathcal{U}_{\rho_c}, \mathcal{U}_{\rho} := \{x \in \phi_{uc} \mid W_c(x) \leq \rho \leq \rho_c\} \subset \mathcal{U}_{\rho_c}, \forall t \geq 0$ .

In addition, it remains to show that for the other initial states  $x_0 \in \phi_{uc} \setminus (\mathcal{D} \cup \mathcal{U}_{\rho_c}), x(t) \notin \mathcal{D}, \forall t \geq 0$  also holds. Given an initial state  $x_0 \in \phi_{uc} \setminus (\mathcal{D} \cup \mathcal{U}_{\rho_c}), W_c(x_0) > \rho_c$  holds. Based on the definition of  $\phi_{uc}$ , it is trivial to show that  $\dot{W}_c(x)$  is still nonpositive  $(\dot{W}_c(x) = 0 \text{ at the origin and } x_e)$  along the trajectory of x(t) under the controller  $u = \Phi(x)$ . Also, from the condition of Eq. (2d) that the set  $\phi_{uc} \setminus (\mathcal{D} \cup \mathcal{U}_{\rho_c})$  does not intersect with  $\overline{\mathcal{D}}$ , we can show that any trajectory starting in  $\phi_{uc} \setminus (\mathcal{D} \cup \mathcal{U}_{\rho_c})$  will reach the boundary of  $\phi_{uc} \setminus (\mathcal{D} \cup \mathcal{U}_{\rho_c}) \cap \overline{\mathcal{D}} = \emptyset$ , it must hold that  $\overline{\phi_{uc}} \setminus (\mathcal{D} \cup \mathcal{U}_{\rho_c}) \cap \mathcal{U}_{\rho_c} \neq \emptyset$ . Therefore, the trajectory will first reach the boundary of  $\phi_{\mu_c} \setminus (\mathcal{D} \cup \mathcal{U}_{\rho_c})$  and enter and stay in  $\mathcal{U}_{\rho_c}$  thereafter.

## 2.5. Lyapunov-based EMPC

The LEMPC scheme is given as follows:

$$\max_{u(t)\in S(\Delta)} \int_{t_k}^{t_{k+N}} L_e(\tilde{x}(\tau), u(\tau)) d\tau$$
(5a)

s.t. 
$$\tilde{\tilde{x}}(t) = f(\tilde{x}(t)) + g(\tilde{x}(t))u(t)$$
 (5b)  
 $u(t) \in U, \quad \forall t \in [t_k, t_{k+N})$  (5c)

$$\tilde{x}(t_k) = x(t_k) \tag{5d}$$

$$V(\tilde{\mathbf{x}}(t)) \le \rho_e, \text{ if } \mathbf{x}(t_k) \in \Omega_{\rho_e},$$
  
$$\forall t \in [t_k, t_{k+N})$$
(5e)

$$\dot{V}(x(t_k), u(t_k)) \leq \dot{V}(x(t_k), \Phi(x(t_k))),$$
  
if  $x(t_k) \in \Omega_{\rho} \setminus \Omega_{\rho_{\rho}}$  (5f)

where  $\tilde{x}$  is the predicted state trajectory,  $S(\Delta)$  is the set of piecewise constant functions with period  $\Delta$ , and N is the number of sampling periods in the prediction horizon.  $\dot{V}(x, u)$  is used to represent

 $\frac{\partial V(x)}{\partial x}(f(x) + g(x)u). \ \Omega_{\rho} \text{ is a level set of } V(x) \text{ inside } \phi_u: \Omega_{\rho} := \{x \in \phi_u \mid V(x) \leq \rho\}, \text{ where } \phi_u \text{ is characterized as the set } \phi_u := \{x \in \mathbb{R}^n \mid u = \Phi(x) \in U, \ V + \gamma V(x) \leq 0, \gamma > 0\} \text{ such that the origin is rendered asymptotically stable if } x_0 \in \Omega_{\rho}. \text{ Additionally,} \\ \Omega_{\rho_e} := \{x \in \phi_u \mid V(x) \leq \rho_e, \rho_e < \rho\} \text{ is also designed to make } \Omega_{\rho} \\ \text{a forward invariant set. The optimal input trajectory computed by the LEMPC is denoted by <math>u^*(t)$ , which is calculated over the entire prediction horizon  $t \in [t_k, t_{k+N})$ . The control action computed for the first sampling period of the prediction horizon is sent by the LEMPC to be applied over the first sampling period and the LEMPC is resolved at the next sampling time.

**Remark 1.** Under the LEMPC of Eq. (5) applied in a sample-andhold fashion, the closed-loop stability of the system of Eq. (1) is guaranteed in the sense that the state x(t),  $t \ge 0$  of the closedloop system of Eq. (1) is always bounded in  $\Omega_{\rho}$  if  $x_0 \in \Omega_{\rho}$ . The detailed proof can be found in [1]. However, it should be pointed out that under the LEMPC of Eq. (5), process operational safety is not ensured because there is no constraint that prevents the state from entering the unsafe region  $\mathcal{D}$ . Although there exist methods (e.g., adding a safety-based constraint in LEMPC such that the predicted closed-loop state is restricted to the safe region [7]), it could lead to the problem of infeasibility.

#### 3. Main results

 $\forall x$ 

#### 3.1. Design of constrained CLBF

Based on the methods for constructing an unconstrained CLBF from [12], in this subsection, the constructive methods for a constrained CLBF are developed. Specifically, a CLF and a CBF are first designed separately for  $x \in \mathbb{R}^n$ , following which a constrained CLBF can be constructed by combining them through a practical method that satisfies the properties in Eq. (2) and Eq. (3). The resulting CLBF  $W_c(x)$  can then be utilized to characterize  $\phi_{uc}$  and  $U_{\rho_c}$ . Proposition 2 provides the guidelines for choosing the CLF and CBF, and the corresponding weights to design the appropriate CLBF, through which the global minimum of  $W_c(x)$  is at the origin.

**Proposition 2.** Given an open set  $\mathcal{D}$  of unsafe states for the nominal system of Eq. (1) with  $w(t) \equiv 0$ , assume that there exists a  $C^1$  CLF  $V : \mathbf{R}^n \to \mathbf{R}_+$ , and a  $C^1$  CBF  $B : \mathbf{R}^n \to \mathbf{R}$ , such that the following conditions hold:

$$c_1|x|^2 \le V(x) \le c_2|x|^2, \ \forall x \in \mathbf{R}^n, \ c_2 > c_1 > 0$$
 (6)

$$\mathcal{D} \subset \mathcal{H} \subset \phi_{uc}, \ \mathbf{0} \notin \mathcal{H} \tag{7}$$

$$B(x) = -\eta < 0, \ \forall x \in \mathbf{R}^n \setminus \mathcal{H}$$
(8)

$$B(x) \ge -\eta, \ \forall x \in \mathcal{H}; \ B(x) > 0, \ \forall x \in \mathcal{D}$$
 (9)

where  $\mathcal{H}$  is a compact and connected set within  $\phi_{uc}$ . Define CLBF  $W_c(x)$  to have the form  $W_c(x) := V(x) + \mu B(x) + \nu$ , where:

$$L_f W_c(x) < 0,$$
  

$$\in \{ z \in \phi_{uc} \setminus (\mathcal{D} \cup \{0\} \cup \mathcal{X}_e) \mid L_g W_c(z) = 0 \}$$
(10a)

$$\left|\frac{\partial W_c(x)}{\partial x}\right| \le \alpha_4(|x|) \tag{10b}$$

$$\mu > \frac{c_2 c_3 - c_1 c_4}{n}, \ \nu = \rho_c - c_1 c_4, \tag{11a}$$

$$c_3 := \max_{x \in \partial \mathcal{H}} |x|^2, \ c_4 := \min_{x \in \partial \mathcal{D}} |x|^2$$
(11b)

then for initial states  $x_0 \in \phi_{uc} \setminus \mathcal{D}_{\mathcal{H}}$ , where  $\mathcal{D}_{\mathcal{H}} := \{x \in \mathcal{H} \mid W_c(x) > \rho_c\} \supset \mathcal{D}$ , the control law  $\Phi(x)$  guarantees that the closed-loop state does not enter the unsafe region  $\mathcal{D}_{\mathcal{H}}$  for all times, and the closed loop state is always bounded in  $\mathcal{U}_{\rho_c}$  for initial states  $x_0 \in \mathcal{U}_{\rho_c}$ .

**Proof.** We define a new compact and connected set  $\mathcal{H}$ , which satisfies Eq. (7), and an expanded unsafe region  $\mathcal{D}_{\mathcal{H}}$ , such that all the states with  $W_c(x) > \rho_c$  inside the region  $\mathcal{H}$  are included in  $\mathcal{D}_{\mathcal{H}}$ . We prove that the proposed constrained CLBF,  $W_c(x)$ , meets all the requirements of Eq. (2) and Eq. (3) with  $\mathcal{D}_{\mathcal{H}}$  replacing  $\mathcal{D}$  and that its minimum is at the origin. If the resulting  $W_c(x)$  satisfies Eq. (2) and has a minimum at the origin with  $\mathcal{D}_{\mathcal{H}}$  replacing  $\mathcal{D}$ , from Theorem 1, it is guaranteed that the closed-loop state does not enter the unsafe region  $\mathcal{D}_{\mathcal{H}}$  for  $x_0 \in \phi_{uc} \setminus \mathcal{D}_{\mathcal{H}}$  under the controller  $u = \Phi(x) \in U$  with the above CLBF  $W_c(x)$ . As a result, it is also guaranteed that the trajectory of the closed-loop system of Eq. (1) avoids  $\mathcal{D}$  due to the fact that  $\mathcal{D} \subset \mathcal{D}_{\mathcal{H}}$ .



**Fig. 1.** A schematic representing the relationship between the sets  $\phi_{uc}$ ,  $\mathcal{D}$ ,  $\mathcal{D}_{\mathcal{H}}$  and  $\mathcal{H}$ , where the invariant set  $\mathcal{U}_{\rho_c}$  is shown as an ellipse subtracting  $\mathcal{D}_{\mathcal{H}}$ .

Firstly, the assumption that  $W_c(x)$  has a minimum at the origin is satisfied since the minimum values of V(x) and B(x) are both achieved at the origin of state-space, respectively and  $W_c(x)$  is formulated through the weighted average of V(x) and B(x). Additionally, we need to prove that the resulting  $W_c(x)$  satisfies the definition of the CLBF of Eq. (2) with  $\mathcal{D}$  replaced by  $\mathcal{D}_{\mathcal{H}}$ . It is trivial to show that Eq. (2a) holds with  $\mathcal{D}$  replaced by  $\mathcal{D}_{\mathcal{H}}$  by the definition of  $\mathcal{D}_{\mathcal{H}}$ . Eq. (2b) is also trivially satisfied by the proposed CLBF  $W_c(x)$ with  $\mathcal{D}_{\mathcal{H}}$  replacing  $\mathcal{D}$  via the required property of Eq. (10a) since  $\mathcal{D}$  is a subset of  $\mathcal{D}_{\mathcal{H}}$ . To prove that Eq. (2c) holds, we obtain the following inequalities for all  $x \in \partial \mathcal{H}$ ,

$$W_{c}(x) = V(x) + \mu B(x) + \nu \leq c_{2}|x|^{2} - \mu \eta + \rho_{c} - c_{1}c_{4} < \rho_{c}$$
(12)

Hence, Eq. (12) implies that  $\mathcal{U}_{\rho_c} \neq \emptyset$ , from which the condition of Eq. (2c) is also satisfied. Since  $W_c(x) = \rho_c$ ,  $\forall x \in \partial \mathcal{D}_{\mathcal{H}}$  and  $W_c(x) < \rho_c$ ,  $\forall x \in \partial \mathcal{H}$ , it implies that  $\mathcal{D}_{\mathcal{H}}$  is in the interior of  $\mathcal{H}$  and that  $\partial \mathcal{H} \cap \partial \mathcal{D}_{\mathcal{H}} = \emptyset$ . Additionally, the relationship among  $\mathcal{D}_{\mathcal{H}}$ ,  $\mathcal{H}$ and  $(\mathcal{D}_{\mathcal{H}} \cup \mathcal{U}_{\rho_c})$  is obtained as follows:  $\mathcal{D} \subset \mathcal{D}_{\mathcal{H}} \subset \mathcal{H} \subset (\mathcal{D}_{\mathcal{H}} \cup \mathcal{U}_{\rho_c})$ , from which it is obvious that the boundary of  $\phi_{uc} \setminus (\mathcal{D}_{\mathcal{H}} \cup \mathcal{U}_{\rho_c})$ does not intersect with the boundary of  $\mathcal{D}_{\mathcal{H}}$  (i.e., Eq. (2d) holds with  $\mathcal{D}$  replaced by  $\mathcal{D}_{\mathcal{H}}$ ,  $\phi_{uc} \setminus (\mathcal{D}_{\mathcal{H}} \cup \mathcal{U}_{\rho_c}) \cap \overline{\mathcal{D}_{\mathcal{H}}} = \emptyset$ ). A schematic describing the above relationship among different sets is shown in Fig. 1. Therefore, it is proved that the above constructing method of  $W_c(x)$  satisfies all the requirements of Eq. (2) with  $\mathcal{D}$  replaced by  $\mathcal{D}_{\mathcal{H}}$ .

Next, we prove that the resulting  $W_c(x)$  also satisfies the assumptions of the CLBF of Eq. (3), which is required in the formulation of CLBF-EMPC and will be used in its proofs later. From Eqs. (6), (8) and (9), the minimums of V(x) and B(x) are V(0) = 0 and  $B(x) = -\eta$ ,  $\forall x \in \mathbf{R}^n \setminus \mathcal{H} \supset \{0\}$  (note that this implies that the minimum value of B(x), which is  $-\eta$  according to Eqs. (8) and (9), occurs at the origin of the state-space). It follows that the global minimum of  $W_c(x)$  is  $W_c(0) = \rho_0 = v - \mu\eta$ , and it holds that  $W_c(x) - \rho_0 > 0$ ,  $\forall x \in \mathbf{R}^n \setminus \{0\}$ . Hence, there exist two class  $\mathcal{K}$  functions  $\alpha_1(|x|)$  and  $\alpha_2(|x|)$  that satisfy Eq. (3a). Additionally, Eq. (3b) and Eq. (3c) are also trivially satisfied  $\forall x \in \phi_{uc} \setminus \mathcal{D}$  by the proposed CLBF via the controller  $u = \Phi(x) \in U$  and the required property of Eq. (10b), respectively.

**Remark 2.** If the unsafe region  $\mathcal{D}$  is characterized as a set that is not entirely inside the stability region, the above constructive method of a CLBF can still be applied via choosing a subset of  $\mathcal{U}_{\rho c}$  as the operating region or defining a smaller unsafe region which is inside the stability region as the new  $\mathcal{D}$ .

#### 3.2. CLBF-based EMPC formulation

The CLBF-EMPC design is represented by the following optimization problem:

$$\max_{u(t)\in S(\Delta)} \int_{t_k}^{t_{k+N}} L_e(\tilde{x}(\tau), u(\tau)) d\tau$$
(13a)

s.t. 
$$\tilde{\tilde{x}}(t) = f(\tilde{x}(t)) + g(\tilde{x}(t))u(t)$$
 (13b)

$$\begin{aligned} x(t_k) &= x(t_k) \\ u(t) &\in U, \ \forall \ t \in [t_k, t_{k+N}) \end{aligned}$$
(13d)

$$W_{c}(\tilde{x}) \leq \rho_{e}, \text{ if } x(t_{k}) \in \mathcal{U}_{\rho_{e}},$$
(15d)

$$t \in [t_k, t_{k+N}) \tag{13e}$$

$$W_c(\mathbf{x}(t_k), \mathbf{u}(t_k)) \le W_c(\mathbf{x}(t_k), \boldsymbol{\Phi}(\mathbf{x}(t_k))),$$
  
if  $\mathbf{x}(t_k) \in \mathcal{U}_{\rho} \setminus \mathcal{U}_{\rho_{\rho}}$  (13f)

where the notation follows that in Eq. (5). The optimization problem of Eq. (13) optimizes the time integral of the stage cost function  $L_e(x(t), u(t))$  of Eq. (13a) subject to the nominal process model of Eq. (13b). Eq. (13c) defines the initial condition for the optimization problem of Eq. (13) using the measurement of the process state at the current time  $t_k$ . Eq. (13d) defines the input constraints applied over the prediction horizon. If  $x(t_k)$  is inside  $\mathcal{U}_{\rho_e}$ , the Mode 1 constraint of Eq. (13e) is applied to maintain the predicted closedloop state within the set  $\mathcal{U}_{\rho_e} \subset \mathcal{U}_{\rho}$ , which is designed to make the safe operating region  $\mathcal{U}_{\rho}$  a forward invariant set and also include the states  $x_e \in \mathcal{X}_e$  inside (i.e.,  $\mathcal{B}_{\delta}(x_e) \subset \mathcal{U}_{\rho_e}$  where  $\delta$  is a sufficiently small positive real number). Under the Mode 2 constraint of Eq. (13f), the contractive constraint is activated only for the first sampling step to decrease the value of  $W_c(x)$ , such that the closedloop state will move back into  $U_{\rho_e}$  within finite sampling steps. The CLBF-EMPC is implemented in a sample-and-hold fashion, and only the first step of the optimized input trajectory will be applied over the next sampling period.

Before we demonstrate closed-loop stability and safety under CLBF-EMPC (Theorem 5), we first establish the following useful propositions. Specifically, Proposition 3 gives the upper bound on the difference between the evolutions of the trajectories of the nominal system (i.e.,  $w(t) \equiv 0$ ) and the disturbed system of Eq. (1). Proposition 4 establishes the relationship of the disturbance bound, Lipschitz constants, and the sampling period that is required to maintain  $\dot{W}_c$  negative during one sampling period, which will be utilized in the proof of closed-loop stability and safety of the CLBF-EMPC in Theorem 5. Also, it should be pointed out that for the CLBF-EMPC of Eq. (13), we omit the case where  $x_0 \in \phi_{uc} \setminus (\mathcal{D} \cup \mathcal{U}_{\rho_c})$  and only consider the initial condition  $x_0 \in \mathcal{U}_\rho \subset \mathcal{U}_{\rho_c}$  since closed-loop stability under CLBF-EMPC represents the boundedness of the state x(t) within an invariant set  $\mathcal{U}_\rho$ .

**Proposition 3.** Consider the system  $\dot{x} = F(x, u, w)$  of Eq. (1) and the nominal system  $\hat{x} = F(\hat{x}, u, 0)$  (i.e.,  $w(t) \equiv 0$ ) with initial conditions  $x_0 = \hat{x}_0 \in U_\rho \subset U_{\rho_c}$ . There exists a class  $\mathcal{K}$  function  $f_w(\cdot)$  and a positive constant  $\beta$  such that the following inequalities hold  $\forall x, \hat{x} \in U_\rho$  and  $w(t) \in W$ :

$$|\mathbf{x}(t) - \hat{\mathbf{x}}(t)| \le f_w(t) := \frac{L_w \theta}{L_x} (e^{L_x t} - 1)$$
(14a)

$$W_{c}(x) \le W_{c}(\hat{x}) + \alpha_{4}(\alpha_{1}^{-1}(\rho - \rho_{0}))|x - \hat{x}| + \beta |x - \hat{x}|^{2}$$
(14b)

**Proof.** Let the error vector  $e(t) = x(t) - \hat{x}(t)$ . The derivative of e(t) can be obtained as follows:

$$|\dot{e}(t)| = |F(x(t), u(t), w(t)) - F(\hat{x}(t), u(t), 0)|$$
(15)

Following Eq. (4a), it is obtained that

$$|\dot{e}(t)| \le L_{x}|x(t) - \hat{x}(t)| + L_{w}|w(t)| \le L_{x}|e(t)| + L_{w}|\theta|$$
(16)

Therefore, for all x(t),  $\hat{x}(t) \in \mathcal{U}_{\rho}$ ,  $|w(t)| \leq \theta$  and zero initial condition (i.e., e(0) = 0), we can derive the upper bound of the norm of the error vector as follows:

$$|e(t)| = |x(t) - \hat{x}(t)| \le \frac{L_w \theta}{L_x} (e^{L_x t} - 1)$$
(17)

Subsequently, we prove Eq. (14b) holds for all  $x, \hat{x} \in U_{\rho}$  by using the Taylor series expansion of  $W_c(x)$  around  $\hat{x}$  as follows:

$$W_c(x) \le W_c(\hat{x}) + \frac{\partial W_c(\hat{x})}{\partial x} |x - \hat{x}| + \beta |x - \hat{x}|^2$$
(18)

Substituting Eq. (3a) and Eq. (3c) into Eq. (18), it follows that

$$W_{c}(x) \le W_{c}(\hat{x}) + \alpha_{4}(\alpha_{1}^{-1}(\rho - \rho_{0}))|x - \hat{x}| + \beta |x - \hat{x}|^{2}$$
(19)

**Proposition 4.** Consider the system of Eq. (1) under the controller  $u = \Phi(x) \in U$ , designed based on  $W_c$  with its minimum at the origin and meeting Eq. (2) and Eq. (3), implemented in sample-and-hold. Let  $\epsilon_w > 0$ ,  $\Delta^* > 0$ ,  $\rho > \rho_e$  satisfy

$$-\alpha_3(\alpha_2^{-1}(\rho_e - \rho_0)) + L'_x M \Delta^* + L'_w \theta \le -\epsilon_w / \Delta^*$$
(20)

where  $\alpha_3(\cdot)$  is a class  $\mathcal{K}$  function such that  $\frac{\partial W_c(x)}{\partial x}F(x, \Phi(x), 0) \leq -\alpha_3(|x|)$  holds for  $x \in \mathcal{U}_{\rho} \setminus \mathcal{U}_{\rho_e}$ . Then, for any  $x(t_k) \in \mathcal{U}_{\rho} \setminus \mathcal{U}_{\rho_e}$ , the following inequality holds:

$$W_c(\mathbf{x}(t)) \le W_c(\mathbf{x}(t_k)), \ \forall t \in [t_k, t_{k+1})$$

$$(21)$$

**Proof.** Assuming  $x(t_k) \in U_{\rho} \setminus U_{\rho_e}$ , we prove that within one sampling period, the value of  $W_c(x)$  is decreasing under the controller  $u(t) = \Phi(x(t_k)) \in U$ . The time derivative of the CLBF  $W_c(x)$  along the trajectory x(t) of the nominal system of Eq. (1) in  $t \in [t_k, t_{k+1})$  is given by

$$\dot{W}_{c}(\mathbf{x}(t)) = \frac{\partial W_{c}(\mathbf{x}(t))}{\partial \mathbf{x}} F(\mathbf{x}(t), \Phi(\mathbf{x}(t_{k})), w(t))$$
(22)

Adding  $\frac{\partial W_c(x(t_k))}{\partial x}F(x(t_k), \Phi(x(t_k)), 0)$  to both sides and using Eq. (3b), the following inequality is obtained:

$$\dot{W}_{c}(x(t)) \leq -\alpha_{3}(|x(t_{k})|) + \frac{\partial W_{c}(x(t))}{\partial x}F(x(t), \Phi(x(t_{k})), w(t)) - \frac{\partial W_{c}(x(t_{k}))}{\partial x}F(x(t_{k}), \Phi(x(t_{k})), 0)$$
(23)

Based on the inequalities of Eq. (3a), Eq. (4b) and the fact that  $|F(x, u, w)| \leq M, \forall x \in U_{\rho}$ , for a constant M > 0, due to the compactness of  $U_{\rho}$ , U, and W, the upper bound of  $\dot{W}_{c}(x(t))$  is derived:

$$\dot{W}_{c}(\mathbf{x}(t)) \leq -\alpha_{3}(\alpha_{2}^{-1}(\rho_{e}-\rho_{0})) + L'_{x}|\mathbf{x}(t)-\mathbf{x}(t_{k})| + L'_{w}\theta$$
  
$$\leq -\alpha_{3}(\alpha_{2}^{-1}(\rho_{e}-\rho_{0})) + L'_{x}M\Delta^{*} + L'_{w}\theta$$
(24)

Therefore, if Eq. (20) is satisfied,  $\dot{W}_c(x(t)) \leq -\epsilon_w / \Delta^*$  holds for all  $x(t_k) \in U_\rho \setminus U_{\rho_e}$ ,  $t \in [t_k, t_{k+1})$ . Through the integral of the above equation, we obtain that  $W_c(x(t_{k+1})) \leq W_c(x(t_k)) - \epsilon_w$ , and also the conclusion shown in Eq. (21).

Based on the CLBF-EMPC of Eq. (13), the following theorem establishes that under the sample-and-hold implementation of the solution of the CLBF-EMPC of Eq. (13), the controller maintains closed-loop stability and safety and the optimization problem is recursively feasible.

**Theorem 5.** Consider the system of Eq. (1) with a constrained CLBF  $W_c(x)$ :  $\mathbb{R}^n \to \mathbb{R}$  that has its minimum at the origin and meets Eqs. (2)

and (3). Let  $\Delta \leq \Delta^*$ ,  $\rho > \rho_e$  satisfy Eq. (20) and  $\rho_e$  be determined as follows:

$$\rho_e \le \rho - \alpha_4 (\alpha_1^{-1}(\rho - \rho_0)) f_w(\Delta) - \beta (f_w(\Delta))^2$$
(25)

Given any initial state  $x_0 \in U_\rho$ , it is guaranteed under the CLBF-EMPC of Eq. (13),  $x(t) \in U_\rho$ ,  $\forall t \ge 0$  for the closed-loop system of Eq. (1), where  $U_\rho \subset U_{\rho_c}$  and  $U_\rho \cap \mathcal{D} = \emptyset$ .

**Proof.** To prove closed-loop stability and safety of the system of Eq. (1) subject to small bounded disturbances (i.e.,  $|w(t)| \leq \theta$ ) under the CLBF-EMPC, we first prove that under the Mode 1 constraint of Eq. (13e) of CLBF-EMPC, the closed-loop state is always bounded in the stability and safety region  $U_{\rho}$  (stability comes from the invariance of the level set of  $W_c(x)$  while safety is due to the fact that  $U_{\rho} \cap D = \emptyset$ ). We then prove that if the system operates in the second operation mode (i.e., the Mode 2 constraint of Eq. (13f) is activated when  $x(t_k) \in U_{\rho} \setminus U_{\rho_e}$ ), the closed-loop state will move towards the origin, and enter  $U_{\rho_e}$  in finite sampling steps. Finally, we prove that the CLBF-EMPC of Eq. (13) is solved with recursive feasibility for all states  $x(t) \in U_{\rho}$ .

*Part* 1: We prove that if  $x(t_k) \in U_{\rho_e}, t_k \geq 0$ , the closed-loop state  $x(t) \in U_{\rho}, \forall t \in [t_k, t_{k+1}]$  holds. Since the state  $x(t_k)$  at  $t = t_k$  is assumed to be in the set  $\mathcal{U}_{\rho_e}$ , the CLBF-EMPC of Eq. (13) operates in the first operation mode (i.e., the Mode 1 constraint of Eq. (13e) is applied and the Mode 2 constraint of Eq. (13f) is inactivated). Initially, we consider the case where the CLBF-EMPC of Eq. (13) is designed using the nominal system, and also applied to the nominal system of Eq. (1). Since the prediction model and the real model are both the nominal system with  $w(t) \equiv 0$ , from the constraint of Eq. (13e), it is trivial to show that  $W_c(\hat{x}(t_{k+1})) \leq t_c(x_k)$  $\rho_e < \rho$  for the nominal system of Eq. (1) where again,  $\hat{x}$  denotes the state of the nominal system. However, if the CLBF-EMPC is designed using the nominal system, but applied to the system of Eq. (1) subject to small bounded disturbances  $|w(t)| \leq \theta$ , from the constraint of Eq. (13e), the predicted state is still within  $\mathcal{U}_{\rho_{e}}$ (i.e.,  $W_c(\hat{x}(t_{k+1})) \leq \rho_e$ ). By Propositions 3 and 4 and Eq. (25), it follows that

$$W_{c}(x(t_{k+1})) \leq \alpha_{4}(\alpha_{1}^{-1}(\rho - \rho_{0}))|x(t_{k+1}) - \hat{x}(t_{k+1})| + \beta |x(t_{k+1}) - \hat{x}(t_{k+1})|^{2} + W_{c}(\hat{x}(t_{k+1})) \leq \alpha_{4}(\alpha_{1}^{-1}(\rho - \rho_{0}))f_{w}(\Delta) + \beta (f_{w}(\Delta))^{2} + \rho_{e} \leq \rho$$
(26)

Therefore, if  $x(t_k) \in U_{\rho_e}$ ,  $x(t_{k+1})$  is always bounded in  $U_\rho$  for both the nominal system of Eq. (1) and the system of Eq. (1) subject to bounded disturbances. Additionally, it is trivial to show that the above inequality holds for any  $t \in [t_k, t_{k+1})$  if we plug in a smaller sampling period into the monotonically increasing function  $f_w(\cdot)$  in Eq. (26).

*Part* 2: In this part, we prove that if  $x(t_k) \in U_\rho \setminus U_{\rho_e}$ , the closed-loop state x(t) will move towards the origin within the next sampling period (i.e.,  $W_c(x(t)) \leq W_c(x(t_k)), \forall t \in [t_k, t_{k+1})$ ), and will enter  $U_{\rho_e}$  within finite sampling steps. Since it is assumed that  $x(t_k) \in U_\rho \setminus U_{\rho_e}$ , the Mode 2 constraint of Eq. (13f) is activated in this case and the Mode 1 constraint of Eq. (13e) remains inactive. Similarly, we first consider the scenario that both the prediction model and the real model are the nominal system of Eq. (1) with  $w(t) \equiv 0$ . From the constraint of Eq. (13f) and Eq. (3b), the following inequality is obtained:

$$\dot{W}_{c}(x(t_{k}), u(t_{k})) = \frac{\partial W_{c}(x(t_{k}))}{\partial x} F(x(t_{k}), u(t_{k}), 0)$$

$$\leq \frac{\partial W_{c}(x(t_{k}))}{\partial x} F(x(t_{k}), \Phi(x(t_{k})), 0)$$

$$\leq -\alpha_{3}(|x(t_{k})|)$$
(27)

where  $u(t_k)$  is the optimal input derived by the CLBF-EMPC at  $t = t_k$ , and applied at the next sampling period (i.e.,  $\forall t \in [t_k, t_{k+1})$ ). Under the sample-and-hold implementation of the CLBF-EMPC of Eq. (13),  $\dot{W_c}(x(t))$ ,  $\forall t \in [t_k, t_{k+1})$  is derived using results similar to Eq. (23) and Eq. (24) by letting w(t) = 0:

$$\dot{W}_{c}(x(t), u(t_{k})) = \frac{\partial W_{c}(x(t))}{\partial x} F(x(t), u(t_{k}), 0)$$

$$\leq -\alpha_{3}(|x(t_{k})|) + L'_{x}M\Delta + L'_{w}|0|$$
(28)

Correspondingly, we can also derive the upper bound for  $\dot{W}_c(x(t), u(t_k))$  for the case that the CLBF-EMPC is designed using the nominal system of Eq. (1) but applied to the system of Eq. (1) subject to bounded disturbances. The results are shown as follows:

$$\dot{W}_{c}(x(t), u(t_{k})) = \frac{\partial W_{c}(x(t))}{\partial x} F(x(t), u(t_{k}), w(t))$$

$$\leq -\alpha_{3}(|x(t_{k})|) + L'_{x} M \Delta + L'_{w} \theta$$
(29)

Since Eq. (20) in Proposition 4 is satisfied, it implies that for both the nominal system of Eq. (1) and the system of Eq. (1) subject to bounded disturbances,  $\dot{W_c}(x(t)) \leq -\epsilon_w/\Delta$ ,  $\forall t \in [t_k, t_{k+1})$  holds, from which we can conclude that  $W_c(x(t)) \leq W_c(x(t_k))$ ,  $\forall t \in [t_k, t_{k+1})$  and  $W_c(x(t_{k+1})) \leq W_c(x(t_k)) - \epsilon_w$  through the integral of  $\dot{W_c}(x(t))$ . Therefore, it follows that within finite sampling steps,  $W_c(x(t))$  will be less than  $\rho_e$ , which implies that the closed-loop state x(t) moves back into  $U_{\rho_e}$ .

So far, we have proved that under the CLBF-EMPC of Eq. (13), whether  $x(t_k) \in U_{\rho_e}$  or  $x(t_k) \in U_{\rho} \setminus U_{\rho_e}$ , the state at the next sampling time  $x(t_{k+1})$  is guaranteed to be bounded in  $U_{\rho}$ . By rolling the horizon, it is trivial to show that x(t),  $t \ge t_k \ge 0$  is always bounded in the stability and safety region  $U_{\rho}$ , which implies that given any initial condition  $x_0 \in U_{\rho}$ , closed-loop stability and process operational safety are guaranteed under the CLBF-EMPC of Eq. (13).

*Part* 3: Lastly, we prove that there exists a feasible solution (i.e., the explicit stabilizing controller  $\Phi(x)$  designed based on  $W_c$  with its minimum at the origin and meeting Eqs. (2) and (3) implemented in sample-and-hold) for the optimization problem of the CLBF-EMPC of Eq. (13) all the time. First, assuming that  $x(t_k) \in U_{\rho_e}$ , the sample-and-hold CLBF-based control law  $u(t) = \Phi(x(t_k + i\Delta))$ ,  $i = 0, 1, \ldots, N - 1$  is a feasible solution to the optimization problem of Eq. (13). Specifically, it satisfies both the input constraint of Eq. (13d) and the constraint of Eq. (13e) (because the state moves towards the origin or the states  $x_e \in U_{\rho_e}$  under  $\Phi(x)$  and thus the predicted states  $\tilde{x}(t_k + i\Delta)$ ,  $i = 0, 1, \ldots, N - 1$  are bounded in  $U_{\rho_e}$ ). On the other hand, if  $x(t_k) \in U_{\rho} \setminus U_{\rho_e}$ , the explicit stabilizing controller  $u(t) = \Phi(x(t_k))$  is also a feasible solution that meets the input constraint of Eq. (13d) and the constraint of Eq. (13f).

After the optimal solution derived from the CLBF-EMPC of Eq. (2) is applied to the next sampling period of the system of Eq. (1) (i.e., the rolling horizon), there still exists a feasible control action for  $x(t_{k+1})$  at  $t = t_{k+1}$  since  $x(t_{k+1}) \in U_{\rho}$  is guaranteed. Again, the solution depends on whether  $x(t_{k+1}) \in U_{\rho_e}$  or  $x(t_{k+1}) \in U_{\rho} \setminus U_{\rho_e}$ , which follows the same two scenarios in the last paragraph. Therefore, the optimization problem of the CLBF-EMPC of Eq. (13) is feasible for all  $x(t) \in U_{\rho}$  if  $x_0 \in U_{\rho}$ .

**Remark 3.** It should be noted that although the CLBF-EMPC of Eq. (13) can be applied to the system of Eq. (1) subject to bounded disturbances, there exists a limit to the bound of disturbances w(t). Typically, the disturbances have to be sufficiently small to satisfy Eq. (20). From Eq. (20), it is easily observed that the terms  $L'_x M \Delta$  and  $L'_w \theta$ , which contain the sampling period  $\Delta$  and the bound on the disturbance  $\theta$ , respectively, are both positive, and therefore

Table 1

Parameter values of the CSTR	
------------------------------	--

$T_0 = 300 \text{ K}$	$F = 5 \text{ m}^3/\text{hr}$
$V = 1 \text{ m}^3$	$E = 5 \times 10^4 \text{ kJ/kmol}$
$k_0 = 8.46 \times 10^6 \text{ m}^3/\text{kmol hr}$	$\Delta H = -1.15 \times 10^4 \text{ kJ/kmol}$
$C_p = 0.231 \text{ kJ/kg K}$	R = 8.314  kJ/kmol K
$\rho_L = 1000 \text{ kg/m}^3$	$C_{A0_s} = 4 \text{ kmol/m}^3$
$Q_s = 0.0 \text{ kJ/hr}$	$C_{A_{\rm s}} = 1.22  {\rm kmol/m^3}$
$T_s = 438 \text{ K}$	

have to be sufficiently small such that there exists a positive  $\epsilon_w$  that satisfies Eq. (20).

**Remark 4.** In the formulation of the CLBF-EMPC of Eq. (13),  $\rho_e$  is determined by Eq. (25) to make  $U_\rho$  a forward invariant set in the presence of small bounded disturbances. Additionally,  $U_{\rho e}$  should be designed to include  $x_e$  where  $\partial W_c(x_e)/\partial x = 0$ . Since when  $x(t_k) \in U_{\rho e}$ , CLBF-EMPC optimizes the control actions to maximize the stage cost function of Eq. (13a) instead of driving the state to the origin or  $x_e$ , the problem of convergence to  $x_e$  is not an issue for the closed-loop system of Eq. (1) under the CLBF-EMPC of Eq. (13). However, if the system is required to be operated at the origin under a tracking MPC,  $W_c(x)$  needs to be well-designed such that  $x_e$  is a saddle point, and an additional constraint needs to be designed in the MPC layer to drive the state away from  $x_e$  in case the state gets trapped in  $x_e$ .

**Remark 5.** Since the economic benefits of CLBF-EMPC depend strongly on the size of the operating region (i.e.,  $U_{\rho}$ ) and in general, a larger  $U_{\rho}$  leads to higher stage costs of Eq. (13a), it is beneficial to expand the operating region over which the CLBF-EMPC is operated (e.g., via a null controllable region (NCR) for nonlinear systems [14]).

#### 4. Application to a chemical process example

A chemical process example is used to illustrate the application of CLBF-EMPC to maintain the closed-loop state within the stability/safety region in state-space. Specifically, a well-mixed, non-isothermal continuous stirred tank reactor (CSTR) where an irreversible second-order exothermic reaction takes place is considered. The reaction transforms a reactant *A* to a product *B* ( $A \rightarrow$ *B*). The inlet concentration of *A*, the inlet temperature and feed volumetric flow rate of the reactor are  $C_{A0}$ ,  $T_0$  and *F*, respectively. The CSTR is equipped with a heating jacket that supplies/removes heat at a rate *Q*. The CSTR dynamic model is described by the following material and energy balance equations:

$$\frac{dC_A}{dt} = \frac{F}{V}(C_{A0} - C_A) - k_0 e^{\frac{-E}{RT}} C_A^2$$
(30a)

$$\frac{dT}{dt} = \frac{F}{V}(T_0 - T) + \frac{-\Delta H}{\rho_L C_p} k_0 e^{\frac{-E}{RT}} C_A^2 + \frac{Q}{\rho_L C_p V}$$
(30b)

where  $C_A$  is the concentration of A in the reactor, V is the volume of the reacting liquid in the reactor, T is the temperature of the reactor and Q is the heat input rate. The concentration of A in the feed is  $C_{A0}$ . The feed temperature and volumetric flow rate are  $T_0$ and F, respectively. The reacting liquid has a constant density of  $\rho_L$ and a heat capacity of  $C_p$ .  $\Delta H$ ,  $k_0$ , E, and R represent the enthalpy of reaction, pre-exponential constant, activation energy, and ideal gas constant, respectively. Process parameter values are listed in Table 1.

The CSTR is initially operated at the steady-state ( $C_{As}$ ,  $T_s$ ) = (1.22 kmol/m<sup>3</sup>, 438 K), and ( $C_{Ao_s} Q_s$ ) = (4 kmol/m<sup>3</sup>, 0 kJ/hr). The manipulated inputs are the inlet concentration of species *A* and the heat input rate, which are represented by the deviation variables



**Fig. 2.** The state-space profiles for the closed-loop CSTR under LEMPC and under the CLBF-EMPC of Eq. (2) for an initial condition (0, 0).

 $\Delta C_{A0} = C_{A0} - C_{A0_s}$ ,  $\Delta Q = Q - Q_s$ , respectively. The manipulated inputs are bounded as follows:  $|\Delta C_{A0}| \le 3.5 \text{ kmol/m}^3$  and  $|\Delta Q| \le 5 \times 10^5 \text{ kJ/hr}$ . Therefore, the states and the inputs of the closed-loop system are  $x^T = [C_A - C_{As} T - T_s]$  and  $u^T = [\Delta C_{A0} \Delta Q]$ , respectively.

The control objective is to maximize the profit of the CSTR process of Eq. (30) while keeping the closed-loop state trajectories in the stability and safety region  $U_{\rho}$  using a CLBF-EMPC scheme. The objective function of the CLBF-EMPC optimizes the production rate of B:  $L_e(\tilde{x}, u) = k_0 e^{-E/RT} C_A^2$ . The unsafe region  $\mathcal{D}$  is defined as an open set inside the stability region (i.e., the level set of V(x)) where the temperature in  $\mathcal{D}$  is relatively high, for this example, an ellipse described by  $\mathcal{D} := \{x \in \mathbb{R}^2 \mid F(x) = (x_1 + 0.92)^2 + \frac{(x_2 - 42)^2}{500} < 0.06\}$ . In general, the unsafe region can be designed based on a real scenario, for example, by using a Safeness Index function proposed by [7] which indicates the relative safeness of each process state based on past process data, first-principles models and traditional safety analysis tools.  $\mathcal{H}$  is defined as  $\mathcal{H} := \{x \in \mathbb{R}^2 \mid F(x) \leq 0.07\}$ , and therefore, the Control Barrier Function B(x) is designed as follows:

$$B(x) = \begin{cases} e^{\frac{F(x)}{F(x) - 0.07}} - e^{-6}, \text{ if } x \in \mathcal{H} \\ -e^{-6}, \text{ if } x \notin \mathcal{H} \end{cases}$$
(31)

A Control Lyapunov Function  $V(x) = x^T P x$  is constructed th  $P = \begin{bmatrix} 1060 & 22\\ 22 & 0.52 \end{bmatrix}$ . Therefore, the Control Lyapunov-Barrier with P =Function  $W_{c}(x) = V(x) + \mu B(x) + \nu$  is constructed following the procedure in Proposition 2, where the parameters are determined as follows:  $\rho_c = 0, c_1 = 0.1, c_2 = 1061, c_3 = \max_{x \in \partial \mathcal{H}} |x|^2 = 2295$ ,  $c_4 = \min_{x \in \partial D} |x|^2 = 1370, v = \rho_c - c_1 c_4 = -160$ . Hence,  $\mu$  is chosen to be  $1 \times 10^9$  to satisfy Eq. (11) and  $\mathcal{U}_{\rho}$  with  $\rho = -2.47 \times 10^6$ is the stability and safety region in the simulation. Based on the above  $W_c(x)$ ,  $x_e$  is calculated to be a saddle point (-1.00, 47.5) in state-space. Additionally, a material constraint  $\frac{1}{t_p} \int_0^{t_p} u_1(\tau) d\tau =$ 0 kmol/m<sup>3</sup> is introduced to make the averaged reactant material available over a given operating period  $t_p = 1.0$  hr to be 0 (in deviation from the steady-state value,  $C_{A0s}$ ). The explicit Euler method with an integration time step of  $h_c = 10^{-4}$  hr is applied to numerically simulate the dynamic model of Eq. (30). The nonlinear optimization problem of the CLBF-EMPC of Eq. (13) is solved using the IPOPT software package [15] with the sampling period  $\Delta$  =  $10^{-2}$  hr. The closed-loop state and manipulated input profiles of the system of Eq. (30) under the CLBF-EMPC of Eq. (13) are shown in Figs. 2 and 3, respectively, where the dashed horizontal lines in Fig. 3 are the upper and lower bounds for the manipulated inputs.

In Fig. 2, it is demonstrated that the CLBF-EMPC can maintain the state of the closed-loop system of Eq. (30) within the stability and safety region (i.e.,  $U_{\rho}$ ), while under the standard LEMPC of Eq. (5), the closed-loop states are only guaranteed to be bounded



**Fig. 3.** Manipulated input profiles  $(u_1 = \Delta C_{A0}, u_2 = \Delta Q)$  for the initial condition (0,0) under the CLBF-EMPC of Eq. (13), and under the LEMPC of Eq. (5).

in the stability region (i.e.,  $U_{\rho} \cup D$ ), but not within the safe region (i.e., it is possible for the trajectory to cross the red unsafe region in Fig. 2). In Fig. 3, it is demonstrated that the optimized control actions satisfy the input constraints and the material constraint. Specifically, under CLBF-EMPC, the control system consumes approximately the maximum allowable reactant  $\Delta C_{A0}$  during the first 0.5 hr, and therefore has to lower the consumption at the second half hour to meet the material constraint. From t = 0.5 hr, the control actions also show oscillation when the closed-loop state approaches the boundary of the unsafe region  $\mathcal{D}$  because the closed-loop system dynamics attempt to drive the states across the unsafe region, yet the CLBF constraint prevents this undesirable behavior. Additionally, it is calculated that the economic benefits  $L_E = \int_0^{t_p} L_e(x, u) dt$  within the entire operation period  $t_p = 1$  hr under steady-state operation and under the CLBF-EMPC are 13.9 and 16.2, respectively, from which it is shown that the CLBF-EMPC economically outperforms steady-state operation and ensures process operational safety.

#### 5. Conclusion

In this work, we proposed a new class of economic model predictive controllers (EMPC) for nonlinear systems that account for process operational safety and economic optimality simultaneously. Specifically, we first developed the constrained Control Lyapunov-Barrier Function. Based on that, the CLBF-EMPC was formulated to achieve economic optimality, safety and closed-loop stability by incorporating CLBF-based constraints in the design of the EMPC. The application of the proposed CLBF-EMPC was demonstrated using a nonlinear chemical process example.

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