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Distributed Economic Model Predictive Control of a Catalytic Reactor: Evaluation of Sequential and Iterative Architectures

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Abstract: The development and application of distributed economic model predictive control (DEMPC) methodologies to a catalytic reactor is considered. Two DEMPC methodologies are designed for sequential and iterative implementation, respectively. The DEMPC architectures are evaluated on the basis of the closed-loop performance and on-line computation time requirements compared to a centralized EMPC approach. For the catalytic reactor considered, DEMPC proves to be a viable option as it is able to give similar closed-loop performance while reducing the on-line computation time requirements relative to a centralized EMPC strategy.

Keywords: Economic model predictive control, distributed model predictive control, process control, nonlinear systems

1. INTRODUCTION

Operating chemical processes in an economically-optimal manner while maintaining closed-loop stability and satisfying the process constraints is an important issue within chemical process control. To accomplish this objective, model predictive control (MPC) has proven to be an attractive way in many industrial applications (e.g., Qin and Badgwell (2003)). MPC is a control methodology that accounts for performance criterion by optimizing a cost function over a finite-time prediction horizon subject to a process model (to predict the future behavior of the process), process constraints, and stability constraints. Traditionally, the cost function used within MPC is a quadratic cost that is positive definite with respect to an operating steady-state of a process.

Given that MPC is implemented in a receding horizon fashion (i.e., an optimization problem is solved on-line at each sampling time to compute the control actions), significant computation delay may result when computing control actions for process systems of high dimension (i.e., many states and inputs) which may affect closed-loop stability and performance. In the context of control of large-scale nonlinear chemical process networks, an alternative is to employ a distributed MPC (DMPC) architecture (e.g., Christofides et al. (2013)). DMPC has the ability to control large-scale multiple-input multiple-output with input and state constraints while remaining computationally feasible to be implemented on-line through a distributed implementation of the computations. Numerous formulations, implementation strategies, and theoretical results have been developed within the context of standard tracking DMPC (e.g, Liu et al. (2009, 2010); see, also, the reviews of Scattolini (2009); Christofides et al. (2013) and the references therein).

To integrate process (dynamic) optimization and control, economic MPC (EMPC), which optimizes a general cost function that represents the process economics instead of a quadratic cost function, has been proposed as a control methodology that may help to enable future manufacturing tasks like demand-driven process operations (e.g., Huang et al. (2011); Angeli et al. (2012); Heidarinejad et al. (2012); see, also, the review Ellis et al. (2014) and the references therein). Recently, significant effort within the control community has focused on (centralized) EMPC. Since EMPC may use a general (nonlinear) economic cost function and may dictate a time-varying operation strategy, the on-line computation required to solve EMPC may be significant especially for large-scale process networks. Thus, distributed EMPC (DEMPC) may be one choice to significantly reduce the on-line computational burden. To date, only a limited amount of work on DEMPC for linear systems [Driessen et al. (2012); Müller and Allgöwer (2014)] and for nonlinear systems [Chen et al. (2012); Lee and Angeli (2012)] has been completed. While these works on distributed EMPC (DEMPC) have shown some promising results on DEMPC, more work in this direction is in order.

In the present work, sequential and iterative distributed EMPC strategies are developed and applied to a benchmark catalytic reactor where time-varying operation of the reactor gives greater yield of the product compared to steady-state operation. A description of the DEMPC

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implementation strategies is provided. Several closed-loop simulations are performed to evaluate the approaches. Two key performance metrics are considered in the evaluation: the closed-loop economic performance under the various DEMPC strategies and the on-line computation time required to solve the EMPC optimization problems.

1.1 Class of Nonlinear Systems

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

$$\dot{x}(t) = f(x(t), u_1(t), \ldots, u_m(t), w(t)) \quad (1)$$

where $x(t) \in R^{n_x}$ denotes the state vector, $u_i(t) \in R^{n_{u_i}}$ for $i = 1, \ldots, m$ denotes the ith manipulated (control) input vector, $w(t) \in R^{n_w}$ denotes the disturbance vector. The (full) input vector has been divided into m input vectors given that m distributed controllers will be designed to control each of the m input vectors. The input vectors are bounded in a convex set denoted as $U_i := \{u_i \in R^{n_{u_i}} \mid u_{ij,\min} \leq u_{ij} \leq u_{ij,\max},\ j = 1, \ldots, n_{u_i}\}$ for $i = 1, \ldots, m$ where $u_{ij,\min}$ and $u_{ij,\max}$ denote the minimum and maximum bound on the jth element of the ith input vector, respectively. Additionally, the disturbance vector is assumed to be bounded: $w(t) \in W := \{w \in R^l \mid |w| \leq \theta\}$ where $\theta > 0$ bounds the norm of the disturbance vector. The vector field of the system of Eq. 1 is assumed to be a locally Lipschitz vector function of its arguments, and the origin of the unforced system is the equilibrium point of Eq. 1 (i.e., $f(0, 0, \ldots, 0, 0) = 0$). A state measurement of the system of Eq. 1 is assumed to be available synchronously at sampling instances denoted as $t_k := t_0 + k\Delta$ where t_0 is the initial time, $k \in I_{\geq 0}$ and $\Delta > 0$ is the sampling period.

1.2 Economic Model Predictive Control

In a centralized approach, one can design an EMPC system that computes control actions for all m input vectors. EMPC, implemented in a centralized approach for the system of Eq. 1, is formulated as follows:

$$\underset{u_1,\ldots,u_m \in S(\Delta)}{\text{maximize}} \quad \int_0^{N\Delta} l_e(\tilde{x}(\tau), u_1(\tau), \ldots, u_m(\tau))\, d\tau \quad (2a)$$

$$\text{subject to} \quad \dot{\tilde{x}}(\tau) = f(\tilde{x}(\tau), u_1(\tau), \ldots, u_m(\tau), 0) \quad (2b)$$

$$\tilde{x}(0) = x(t_k) \quad (2c)$$

$$u_i(\tau) \in U_i,\ \forall\, \tau \in [0, N\Delta) \quad (2d)$$

$$\int_0^{N\Delta} g(\tilde{x}(\tau), u(\tau))\, d\tau \leq 0 \quad (2e)$$

where $i = 1, \ldots, m$ and the notation $S(\Delta)$ denotes the family of piecewise constant functions with period Δ, $\tilde{x}(\tau)$ denotes the predicted state trajectory under the piecewise constant input profiles, $u_1(\tau), \ldots, u_m(\tau)$, which are the decision variable of the dynamic optimization problem, Δ is the sampling period of the EMPC, and N is a positive integer that denotes the prediction horizon (i.e., number of sampling periods in the prediction horizon). To distinguish between real-time and the prediction time of the EMPC, t denotes the real (continuous) time, t_k denotes the discrete sampling instances where state feedback is obtained, and $\tau \in [0, N\Delta)$ denotes the predicted time in the controller.

The stage cost $l_e(x, u_1, \ldots, u_m)$ of the EMPC is one of the design/tuning elements of the EMPC. It is chosen to reflect the process economics and need not be a quadratic stage cost like that typically used with standard tracking MPC. The stage cost of the EMPC is referred to as the economic cost function. The computed input profile optimizes the economic cost (2a) over the prediction horizon while accounting for the following constraints. The constraint (2b) is the dynamic model of the process initialized with a state measurement (2c) received at sampling instance t_k. The nominal dynamic model predicts the future behavior of the process under any input trajectories $u_1(\tau), \ldots, u_m(\tau)$ for $\tau \in [0, N\Delta)$ and allows for the EMPC to compute the optimal input trajectories. The optimal input trajectories are denoted: $u_1^*(\tau|t_k), \ldots, u_m^*(\tau|t_k)$ for $\tau \in [0, N\Delta)$. The bounds on the inputs are given by the constraints of (2d). Lastly, the constraint (2e) represents economics-based constraints which are typically integral constraints.

EMPC, like standard tracking MPC, is implemented in a receding horizon fashion. At a sampling instance t_k, the controller receives the current state measurement $x(t_k)$, computes the optimal input trajectories $u_1^*(\tau|t_k), \ldots, u_m(\tau|t_k)$ for $\tau \in [0, N\Delta)$ (which corresponds from t_k to t_{k+N}), and implements the control action computed for the first sampling period in the prediction horizon on the process: $u_i(t) = u_i^*(0|t_k)$ for $t \in [t_k, t_{k+1})$. The process is repeated at the next sampling time by rolling the horizon one sampling period.

2. CATALYTIC REACTOR EXAMPLE

A catalytic reactor example is considered to evaluate various DEMPC implementation strategies. A non-isothermal continuous stirred tank reactor (CSTR) where ethylene is catalytically converted to ethylene oxide is considered. Besides the oxidation reaction, two combustion reactions occur that consume ethylene and ethylene oxide. The three reactions are given by:

$$C_2H_4 + \frac{1}{2}O_2 \xrightarrow{r_1} C_2H_4O \quad (R1)$$

$$C_2H_4 + 3O_2 \xrightarrow{r_2} 2CO_2 + 2H_2O \quad (R2)$$

$$C_2H_4O + \frac{5}{2}O_2 \xrightarrow{r_3} 2CO_2 + 2H_2O \quad (R3)$$

The reactor has a cooling jacket to remove the heat generated by the three exothermic reactions. The catalytic reactor has three manipulated inputs: the volumetric flow rate of the reactor feed, the ethylene concentration in the reactor feed, and the coolant jacket temperature.

The gaseous mixture contained in the reactor is assumed to be an ideal gas. By employing other standard modeling assumptions, a dynamic model can be developed for the catalytic reactor, and the resulting dynamic model has four states: the reactor gas mixture density, the reactor ethylene concentration, the reactor ethylene oxide concentration, and the reactor temperature. The states are denoted as x_1, x_2, x_3, and x_4, respectively, and the inputs are denoted u_1, u_2, and u_3, respectively (dimensionless variable form is used for all variables). The complete model can be found in Özgülşen et al. (1992) which uses the nonlinear Arrhenius reaction rate laws of Alfani and Carberry (1970). The admissible input values are given by the following sets: