



Distributed economic MPC: Application to a nonlinear chemical process network

Xianzhong Chen^a, Mohsen Heidarinejad^b, Jinfeng Liu^a, Panagiotis D. Christofides^{a,b,*}

^a Department of Chemical and Biomolecular Engineering, University of California, Los Angeles, CA 90095-1592, USA

^b Department of Electrical Engineering, University of California, Los Angeles, CA 90095-1592, USA

ARTICLE INFO

Article history:

Received 28 September 2011
Received in revised form 25 January 2012
Accepted 26 January 2012
Available online 29 February 2012

Keywords:

Nonlinear systems
Model predictive control
Process economics
Process control

ABSTRACT

In the present work, we focus on the development and application of Lyapunov-based economic model predictive control (LEMPC) designs to a catalytic alkylation of benzene process network, which consists of four continuously stirred tank reactors and a flash separator. We initially propose a new economic measure for the entire process network which accounts for a broad set of economic considerations on the process operation including reaction conversion, separation quality and energy efficiency. Subsequently, steady-state process optimization is first carried out to locate an economically optimal (with respect to the proposed economic measure) operating steady-state. Then, a sequential distributed economic model predictive control design method, suitable for large-scale process networks, is proposed and its closed-loop stability properties are established. Using the proposed method, economic, distributed as well as centralized, model predictive control systems are designed and are implemented on the process to drive the closed-loop system state close to the economically optimal steady-state. Extensive simulations are carried out to demonstrate the application of the proposed economic MPC (EMPC) designs and compare them with a centralized Lyapunov-based model predictive control design, which uses a conventional, quadratic cost function that includes penalty on the deviation of the states and inputs from their economically optimal steady-state values, from computational time and closed-loop performance points of view.

© 2012 Elsevier Ltd. All rights reserved.

1. Introduction

The traditional, and currently dominant, approach to the achievement of economic optimization considerations of a plant relies on the use of a two-layer approach in which the upper layer is used to compute optimal process operation points taking into account economic considerations and using steady-state process models, and the lower-layer (i.e., process control layer) employs automatic feedback control systems to force the process to operate at the economically optimal steady-state computed by the upper layer. In the process control layer, classical control schemes wherever appropriate, as well as model predictive control (MPC) due to its ability to deal with multivariable constrained control problems and to account for optimization considerations [7,18], are widely used in industry. In the context of MPC, the standard approach is to use a quadratic cost function that involves penalties on the deviations of the state variables and of the control actions from their economically-optimal steady-state values over a finite prediction horizon. This consideration, together with appropriate

stability constraints, allows standard MPC schemes to drive the state of the closed-loop system to the economically optimal steady-state for a suitable set of initial conditions. While this approach to enforcing economic considerations in the context of standard MPC formulations is widely used, there is room to improve upon the incorporation of economic considerations in the control layer and the computation of the control action.

To this end, there have been several authors within process control advocating the tighter integration of MPC and economic optimization of processes (e.g., [17,1,21,10]). In [9], two economic MPC schemes were proposed for cyclic processes and nominal stability of the closed-loop system was established via Lyapunov techniques. MPC designs using an economics-based cost function were proposed in [5] and the closed-loop stability properties were established via a suitable Lyapunov function through adoption of a terminal constraint which requires that the closed-loop system state is driven to a steady-state at the end of the prediction horizon. Even though a rigorous stability analysis is included in [5], it is difficult, in general, to characterize, a priori, the set of initial conditions starting from where feasibility and closed-loop stability of the proposed MPC scheme are guaranteed. In contrast, in [8], we proposed a Lyapunov-based centralized economic MPC (LEMPC) scheme which has two different operation modes. The first operation mode corresponds to the period in which the cost function should be optimized while the second operation mode corresponds to

* Corresponding author at: Department of Chemical and Biomolecular Engineering, University of California, Los Angeles, CA 90095-1592, USA. Tel.: +1 310 794 1015; fax: +1 310 206 4107.

E-mail address: pdc@seas.ucla.edu (P.D. Christofides).

operation in which the system is driven by the economic MPC to an appropriate ideally economically optimal steady-state. The design proposed in [8] took advantage of the pre-defined Lyapunov-based controller to achieve feasibility and characterize the closed-loop stability region.

All of the above economic MPC designs are centralized in nature, that is the optimal manipulated input trajectories are computed from the solution of a single optimization problem. This approach is clearly effective in a number of applications but it may be limited in the context of large-scale nonlinear process networks that involve a large number of manipulated inputs. Distributed MPC (DMPC) has emerged as a feasible alternative to reduce the computational complexity of centralized MPC by solving multiple, reduced-order optimization problems in a parallel, iterative fashion; the reader may refer to [2,22,15,23,16,4] for recent results in this area. However, all the existing DMPC methods utilize quadratic cost function that penalize the deviation of the states and inputs from their operating steady-state values, and generally, they do not explicitly account for economic objectives.

Motivated by the above, we focus on the development and application of distributed and centralized LEMPC designs to a catalytic alkylation of benzene process network, which consists of four continuously stirred tank reactors and a flash separator. A new economic measure for the entire process network is proposed which accounts for a broad set of economic considerations on the process operation including reaction conversion, separation quality and energy efficiency. Subsequently, steady-state process optimization is first carried out to locate an economically optimal (with respect to the proposed economic measure) operating steady-state. Then, a sequential distributed economic model predictive control design method, suitable for large-scale process networks, is proposed and its closed-loop stability properties are established. Using the proposed method, economic, distributed as well as centralized, model predictive control systems are designed and are implemented on the process to drive the closed-loop system state close to the economically optimal steady-state. The closed-loop performance and time needed for control action calculation are evaluated through simulations and compared with the ones of a centralized Lyapunov-based model predictive control design, which uses a conventional, quadratic cost function that includes penalty on the deviation of the states and inputs from their economically optimal steady-state values.

2. Preliminaries

2.1. Notation

The notation $|\cdot|$ is used to denote the Euclidean norm of a vector, and a continuous function $\alpha : [0, a] \rightarrow [0, \bar{a}]$ is said to belong to class \mathcal{K} if it is strictly increasing and satisfies $\alpha(0) = 0$. The symbol Ω_r is used to denote the set $\Omega_r := \{x \in \mathbb{R}^{n_x} : V(x) \leq r\}$ where V is a scalar continuous differentiable positive definite function, and the operator ' \setminus ' denotes set subtraction, that is, $A \setminus B := \{x \in \mathbb{R}^{n_x} : x \in A, x \notin B\}$. The symbol $\text{diag}(v)$ denotes a matrix whose diagonal elements are the elements of vector v and all the other elements are zeros.

2.2. Class of nonlinear systems

We consider nonlinear systems described by the following state-space model:

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

where $x(t) \in \mathbb{R}^{n_x}$ denotes the vector of state variables of the system, $u_i(t) \in \mathbb{R}^{m_{u_i}}$ ($i = 1, \dots, m$) and $w(t) \in \mathbb{R}^{n_w}$ are the i th set of control (manipulated) inputs and disturbances, respectively. The m sets of inputs are restricted to be in m nonempty convex sets

$U_i \subseteq \mathbb{R}^{m_{u_i}}$, $i = 1, \dots, m$, which are defined as $U_i := \{u_i \in \mathbb{R}^{m_{u_i}} : |u_i| \leq u_i^{\max}\}$ where u_i^{\max} , $i = 1, \dots, m$, are the magnitudes of the input constraints. We will design m controllers to compute the m sets of control inputs u_i , $i = 1, \dots, m$, respectively. We will refer to the controller computing u_i as controller i . $w(t)$ is assumed to be bounded, that is, $w(t) \in W$ with $W := \{w \in \mathbb{R}^{n_w} : |w| \leq \theta, \theta > 0\}$. We assume that f is a locally Lipschitz vector function and that the origin is an equilibrium point of the unforced nominal system (i.e., system of Eq. (1) with $u_i(t) = 0$, $i = 1, \dots, m$, $w(t) = 0$ for all t) which implies that $f(0, \dots, 0) = 0$.

2.3. Stabilizability assumptions

We assume that there exists a feedback controller $h(x) = [h_1(x) \dots h_m(x)]^T$ which renders the origin of the nominal closed-loop system asymptotically stable with $u_i = h_i(x)$, $i = 1, \dots, m$, while satisfying the input constraints for all the states x inside a given stability region. Using converse Lyapunov theorems [14,3], this assumption implies that there exist class \mathcal{K} functions $\alpha_i(\cdot)$, $i = 1, 2, 3, 4$ and a continuously differentiable Lyapunov function $V(x)$ (corresponding to the equilibrium point which is assumed to be the origin here) for the nominal closed-loop system which is continuous and bounded in $O \subseteq \mathbb{R}^{n_x}$ where O is an open neighborhood of the origin, that satisfy the following inequalities:

$$\begin{aligned} \alpha_1(|x|) &\leq V(x) \leq \alpha_2(|x|) \\ \frac{\partial V(x)}{\partial x} f(x, h_1(x), \dots, h_m(x), 0) &\leq -\alpha_3(|x|) \\ \left| \frac{\partial V(x)}{\partial x} \right| &\leq \alpha_4(|x|), \quad h_i(x) \in U_i, \quad i = 1, \dots, m \end{aligned} \quad (2)$$

for all $x \in O$. We denote the region $\Omega_\rho \subseteq O$ (Ω_ρ is a level set of $V(x)$) as the stability region of the closed-loop system under the Lyapunov-based controller $h(x)$. Note that explicit stabilizing control laws that provide explicitly defined regions of attraction for the closed-loop system have been developed using Lyapunov techniques for specific classes of nonlinear systems, particularly input-affine nonlinear systems; the reader may refer to [11,3,13] for results in this area including results on the design of bounded Lyapunov-based controllers by taking explicitly into account constraints for broad classes of nonlinear systems. The Lyapunov-based controller, $h(x)$, will be used as an auxiliary controller in the formulation of the economic distributed MPC in Section 4 below.

By continuity, the local Lipschitz property assumed for the vector field f and taking into account that the manipulated inputs u_i , $i = 1, \dots, m$ are bounded, there exists a positive constant M such that:

$$|f(x, u_1, \dots, u_m, w)| \leq M \quad (3)$$

for all $x \in \Omega_\rho$ and $u_i \in U_i$, $i = 1, \dots, m$. By the continuous differentiable property of the Lyapunov function $V(x)$ and the Lipschitz property assumed for the vector field f , there exist positive constants L_x , L_w , L'_x and L'_w such that:

$$\begin{aligned} |f(x, u_1, \dots, u_m, w) - f(x', u_1, \dots, u_m, 0)| &\leq L_x |x - x'| + L_w |w| \\ \left| \frac{\partial V(x)}{\partial x} f(x, u_1, \dots, u_m, w) - \frac{\partial V(x')}{\partial x} f(x', u_1, \dots, u_m, 0) \right| &\leq L'_x |x - x'| + L'_w |w| \end{aligned} \quad (4)$$

for all $x, x' \in \Omega_\rho$, $u_i \in U_i$, $i = 1, \dots, m$ and $w \in W$.

3. Nonlinear chemical process network

In this section, we initially describe the alkylation of benzene process network. Subsequently, we introduce the economic cost measure.

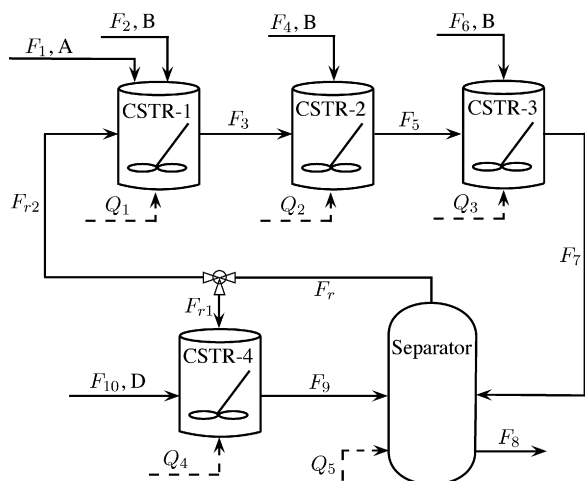


Fig. 1. Process flow diagram of alkylation of benzene.

3.1. Description of the alkylation of benzene process

The process of alkylation of benzene with ethylene to produce ethylbenzene is widely used in the petrochemical industry. Dehydration of the product produces styrene, which is the precursor to polystyrene and many copolymers. Over the last two decades, several modeling and simulation results of alkylation of benzene with catalysts have been reported in the literature. The process model developed in this section is based on Refs. [6,12,20,25,26]. More specifically, the process considered in this work consists of four continuously stirred tank reactors (CSTRs) and a flash tank separator, as shown in Fig. 1. The CSTR-1, CSTR-2 and CSTR-3 are in series and involve the alkylation of benzene with ethylene. Pure benzene is fed through stream F_1 and pure ethylene is fed through streams F_2 , F_4 and F_6 . Two catalytic reactions take place in CSTR-1, CSTR-2 and CSTR-3. Benzene (A) reacts with ethylene (B) and produces the required product ethylbenzene (C) (reaction 1); ethylbenzene can further react with ethylene to form 1,3-diethylbenzene (D) (reaction 2) which is the byproduct. The effluent of CSTR-3, including the products and leftover reactants, is fed to a flash tank separator, in which most of benzene is separated overhead by vaporization and condensation techniques and recycled back to the plant and the bottom product stream is removed. A portion of the recycle stream $F_{r,2}$ is fed back to CSTR-1 and another portion of the recycle stream $F_{r,1}$ is fed to CSTR-4 together with an additional feed stream F_{10} which contains 1,3-diethylbenzene from further distillation process that we do not consider in this example. In CSTR-4, both reaction 2 and the catalyzed transalkylation reaction in which 1,3-diethylbenzene reacts with benzene to produce ethylbenzene (reaction 3) take place. All chemicals left from CSTR-4 eventually pass into the separator. All the materials in the reactions are in liquid phase due to high pressure. The dynamic equations describing the behavior of the process, obtained through material and energy balances under standard modeling assumptions, can be found in [16]. The process model consists of 25 coupled nonlinear ordinary differential equations.

Each of the tanks has an external heat/coolant input. The manipulated inputs to the process are the heat injected to or removed from the five vessels, Q_1 , Q_2 , Q_3 , Q_4 and Q_5 , and the feed streams F_2 , F_4 and F_6 to CSTR-1, CSTR-2 and CSTR-3, respectively. The states of the process consist of the concentrations of A, B, C, D in each of the five vessels and the temperatures of the vessels. The measurement of the process state is assumed to be available continuously to the controllers; i.e., state feedback control is considered.

3.2. Economic cost measure

In this example, we consider the economic measure shown below accounting for three aspects: reaction conversion, separation quality, and energy efficiency:

$$L(x, u_1, \dots, u_m) = A_1 \frac{r_1}{r_2} + A_2 r_3 - A_4 Q_4 - A_5 Q_5 + A_3 \frac{F_8 C_{C4}}{F_8 (C_{A4} + C_{B4} + C_{C4} + C_{D4})} \quad (5)$$

where $L(x, u_1, \dots, u_m)$ is the economic measure, x is the state of the system, u_1, \dots, u_m are the manipulated inputs with $U := [u_1 \dots u_m] = [Q_1 Q_2 Q_3 Q_4 Q_5 F_2 F_4 F_6]$ and A_1, \dots, A_5 are constant weighting coefficients, r_1 , r_2 and r_3 are the reaction rates of reactions 1, 2 and 3, respectively, and C_{A4} , C_{B4} , C_{C4} and C_{D4} are concentrations of species A, B, C, D in the product outlet flow F_8 . Note that the reaction rates are related to the concentrations of the reactants and the temperature in each reactor.

The first two terms of the measure describe the reaction conversion and the goal is to increase the rate of reactions 1 and 3 but suppress the rate of reaction two since it produces a by-product. The third and fourth terms of the measure focus on energy efficiency. The fifth term of the measure takes the separation step into account, and the separation quality is measured in terms of the mole fraction of species C in the outlet stream F_8 . We first solve a steady-state optimization problem using the economic measure of Eq. (5) as the cost function to be maximized to compute an economically optimal operating steady-state. The detailed formulation is shown below:

$$\max_{x, u_1, \dots, u_m} L(x, u_1, \dots, u_m) \quad (6a)$$

$$\text{s.t. } f(x, u_1, \dots, u_m, 0) = 0 \quad (6b)$$

$$u_i \in U_i \quad (6c)$$

$$x \in X \quad (6d)$$

$$\sum_{i=2,4,6} F_i = F^{\max} \quad (6e)$$

$$V(x) \leq \tilde{\rho} \quad (6f)$$

where $L(x, u_1, \dots, u_m)$ is the economic measure in Eq. (5), $f(x, u_1, \dots, u_m, 0)$ is the nominal steady-state process model that described in [16], F^{\max} is the maximum amount of reactant B that is allowed to enter the process per second, and V is a Lyapunov function of the form $V(x) = (x - x^s)^T P (x - x^s)$ with P being a diagonal matrix of the form $\text{diag}([1 \ 10^2 \ 1 \ 10^2 \ 1 \ 10^2 \ 1 \ 10^2 \ 1 \ 10^2 \ 1 \ 10^2 \ 1 \ 10^2 \ 1 \ 10^2 \ 1 \ 10^2 \ 1 \ 10^2 \ 1 \ 10^2])$; the approach that we follow to compute $V(x)$ will be discussed in Remark 2. The optimal solution to this optimization problem is denoted as x^s and u_i^s , $i = 1, \dots, m$.

In the problem of Eq. (6), the constraint of Eq. (6b) guarantees that the optimal solution satisfies the steady-state process model; the constraints of Eqs. (6c) and (6d) define the state and input constraints; the constraint of Eq. (6e) implies that the total amount of feed input B distributed through the stream F_2 , F_4 , and F_6 has to be equal to the maximum feed input F^{\max} ; and, the constraint of Eq. (6f) imposes a Lyapunov constraint so that the solution has to lie inside the level set $\tilde{\rho}$.

We consider the system starting at $t=0$ from a stable steady-state (x_0) that is defined by the steady-state inputs shown in Table 1. The state constraints that are imposed in this example require that the upper and lower bounds of the optimal temperature states are $\pm 6\%$ from the steady-state values of Table 1. The values of the rest of the state variables (concentrations) are required to be positive. The constraints that the manipulated inputs are subjected to are shown in Table 2. The values of F^{\max} and $\tilde{\rho}$ are taken to

Table 1
Steady-state input values.

u_1	-4.4×10^6 [J/s]	u_2	-4.6×10^6 [J/s]
u_3	-4.7×10^6 [J/s]	u_4	9.2×10^6 [J/s]
u_5	5.9×10^6 [J/s]	u_6	8.697×10^{-4} [m ³ /s]
u_7	8.697×10^{-4} [m ³ /s]	u_8	8.697×10^{-4} [m ³ /s]

Table 2
Manipulated input constraints.

$ u_1^s - u_1 \leq 4.0 \times 10^6$ [J/s]	$ u_2^s - u_5 \leq 2.0 \times 10^6$ [J/s]
$ u_2^s - u_2 \leq 4.0 \times 10^6$ [J/s]	$ u_6^s - u_6 \leq 8.679 \times 10^{-4}$ [m ³ /s]
$ u_3^s - u_3 \leq 4.0 \times 10^6$ [J/s]	$ u_7^s - u_7 \leq 8.679 \times 10^{-4}$ [m ³ /s]
$ u_4^s - u_4 \leq 4.0 \times 10^6$ [J/s]	$ u_8^s - u_8 \leq 8.679 \times 10^{-4}$ [m ³ /s]

Table 3
Optimal steady-state input values.

u_1^s	-5.773×10^6 [J/s]	u_2^s	-4.281×10^6 [J/s]
u_3^s	-1.481×10^6 [J/s]	u_4^s	6.238×10^6 [J/s]
u_5^s	7.010×10^6 [J/s]	u_6^s	1.296×10^{-3} [m ³ /s]
u_7^s	7.355×10^{-4} [m ³ /s]	u_8^s	5.773×10^{-4} [m ³ /s]

be 26.091×10^{-4} mol/s and 2.4×10^6 , respectively, and the coefficients A_1, A_2, A_3, A_4, A_5 are chosen to be 3, 1, 45, 27×10^{-7} , and 21×10^{-7} , respectively.

The steady-state optimization problem of Eq. (6) was solved by the open source interior point optimizer Ipopt under default settings in a JAVA programming environment. Simulation results indicate that there is only one optimal solution, and the optimal input values are given in Table 3. We also note that the optimal steady-state is unstable, determined by computing the Jacobian eigenvalues, and some temperature states of the final solution are at the boundary of the set X . The value of the Lyapunov function of the optimal solution of Eq. (6) is 1.45×10^6 , which lies inside the set $\tilde{\rho}$. The optimal value of the economic measure is 33.41, which is a 5.7% increase from the initial steady-state of Table 1, and the weight placed on the various terms of the economic measure is shown in Fig. 2. We note that we nearly-equally weigh reaction conversion (first two terms), energy efficiency (third and fourth terms) and separation (fifth term). This was done because we consider, from a cost point of view, that these three terms equally contribute into the cost but if this is not the case, then the weights can be readily modified to accommodate different cost contributions of each one of these terms.

4. Distributed LEMPC

As the number of manipulated inputs increases as it is the case in the context of control of large-scale chemical plants, the evaluation time of a centralized MPC may increase significantly. This may impede the ability of centralized MPC to carry out real-time

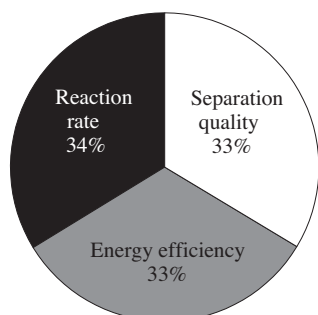


Fig. 2. Weight percentage on the terms of the economic measure used by the steady-state optimization problem.

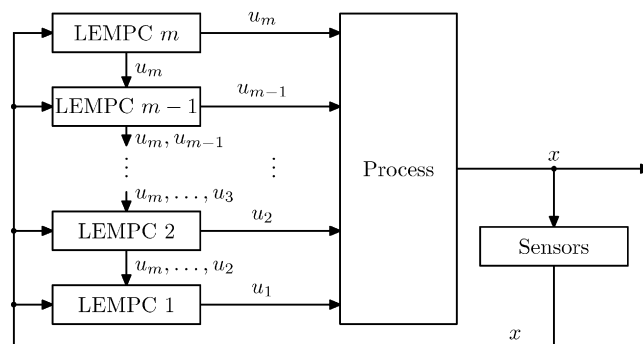


Fig. 3. Distributed LEMPC architecture.

calculations within the limits imposed by process dynamics and operating conditions. Moreover, a centralized control system for large-scale systems may be difficult to organize and maintain and is vulnerable to potential process faults. To overcome these issues, in this work, we propose to utilize a sequential distributed economic model predictive control (EMPC) architecture as shown in Fig. 3. In this architecture, each set of the m sets of control inputs is calculated using an LEMPC. The distributed controllers are connected using one-directional communication network, evaluated in sequence. We will refer to the controller computing u_i associated with subsystem i as LEMPC i . In this section, we propose two different implementation strategies for the sequential distributed EMPC architecture and we assume that the state x of the system is sampled synchronously and the time instants at which we have state measurements are indicated by the time sequence $\{t_{k \geq 0}\}$ with $t_k = t_0 + k\Delta$, $k = 0, 1, \dots$ where t_0 is the initial time and Δ is the sampling time.

4.1. Implementation strategy I

In this implementation strategy for the distributed LEMPC architecture, all the distributed controllers are evaluated in sequence and once at each sampling time. Specifically, at a sampling time, t_k , when a measurement is received, the distributed controllers evaluate their future input trajectories in sequence starting from LEMPC m to LEMPC 1. Once a controller finishes evaluating its own future input trajectory, it sends its own future input trajectory and the future input trajectories it received to the next controller (i.e., LEMPC j sends input trajectories of u_i , $i = m, \dots, j$, to LEMPC $j - 1$).

This implementation strategy implies that LEMPC j , $j = m, \dots, 2$, does not have any information about the values that u_i , $i = j - 1, \dots, 1$ will take when the optimization problem of LEMPC j is solved. In order to make a decision, LEMPC j , $j = m, \dots, 2$ must assume trajectories for u_i , $i = j - 1, \dots, 1$, along the prediction horizon. To this end, the Lyapunov-based controller $h(x)$ is used. In order for the distributed EMPC to inherit the stability properties of the controller $h(x)$, each control input u_i , $i = 1, \dots, m$ must satisfy a constraint that guarantees a given minimum contribution to the decrease rate of the Lyapunov function $V(x)$. Specifically, the proposed design of the LEMPC j , $j = 1, \dots, m$, is based on the following optimization problem:

$$\max_{u_j \in \mathcal{S}(\Delta)} \int_{t_k}^{t_{k+N}} L(\tilde{x}^j(\tau), u_1(\tau), \dots, u_m(\tau)) d\tau \quad (7a)$$

$$\text{s.t. } \dot{\tilde{x}}^j(t) = f(\tilde{x}^j(t), u_1(t), \dots, u_m(t), 0) \quad (7b)$$

$$\begin{aligned} u_i(t) &= h_i(\tilde{x}^j(t_{k+l})), \quad i = 1, \dots, j - 1, \quad \forall t \in [t_{k+l}, t_{k+l+1}), \quad l \\ &= 0, \dots, N - 1 \end{aligned} \quad (7c)$$

$$u_i(t) = u_i^*(t|t_k), \quad i = j + 1, \dots, m \quad (7d)$$

$$u_j(t) \in U_j, \quad i = 1, \dots, m \quad (7e)$$

$$\tilde{x}^j(t_k) = x(t_k) \quad (7f)$$

$$V(\tilde{x}^j(t)) \leq \tilde{\rho}, \quad \forall t \in [t_k, t_{k+N}), \text{ if } t_k \leq t' \text{ and } V(x(t_k)) \leq \tilde{\rho} \quad (7g)$$

$$\begin{aligned} & \frac{\partial V(x(t_k))}{\partial x} f(x(t_k), u_1^n(t_k), \dots, u_{j-1}^n(t_k), u_j(t_k), \dots, u_m(t_k)) \\ & \leq \frac{\partial V(x(t_k))}{\partial x} f(x(t_k), u_1^n(t_k), \dots, u_j^n(t_k), u_{j+1}(t_k), \dots, u_m(t_k)), \text{ if } t_k \\ & > t' \text{ or } \tilde{\rho} < V(x(t_k)) \leq \rho \end{aligned} \quad (7h)$$

where \tilde{x}^j is the predicted trajectory of the nominal system with $u_i, i = j + 1, \dots, m$, the input trajectory computed by the LEMPC controllers of Eq. (7) evaluated before LEMPC j , $u_i, i = 1, \dots, j - 1$, the corresponding elements of $h(x)$ applied in a sample-and-hold fashion, $u_i^*(t|t_k)$ denotes the future input trajectory of u_i obtained by LEMPC i of the form of Eq. (7), and $u_i^n(t_k), i = 1, \dots, m$, are inputs determined by $h_i(x(t_k))$ (i.e., $u_i^n(t_k) = h_i(x(t_k))$). The optimal solution to the optimization problem of Eq. (7) is denoted $u_i^*(t|t_k)$ which is defined for $t \in [t_k, t_{k+N})$. The relation between $\tilde{\rho}$ and ρ is characterized in Theorem 1.

In the optimization problem of Eq. (7), the constraint of Eq. (7g) is only active when $x(t_k) \in \Omega_{\tilde{\rho}}$ in the first operation mode and is incorporated to ensure that the predicted state evolution of the closed-loop system is maintained in the region $\Omega_{\tilde{\rho}}$ (thus, the actual state of the closed-loop system is in the stability region Ω_{ρ} ; this point will be proved in Theorem 1 below). Due to the fact that all of the controllers receive state feedback $x(t_k)$ at sampling time t_k , all of the distributed controllers operate in the same operation mode by verifying whether $V(x(t_k)) \leq \tilde{\rho}$; the constraint of Eq. (7h) is only active in the second operation mode or when $\tilde{\rho} < V(x(t_k)) \leq \rho$ in the first operation mode. This constraint guarantees that the contribution of input u_j to the decrease rate of the time derivative of the Lyapunov function $V(x)$ at the initial time (i.e., t_k), if $u_j = u_j^*(t_k|t_k)$ is applied, is bigger than or equal to the value obtained when $u_j = h_j(x(t_k))$ is applied.

The manipulated inputs of the proposed distributed control design from time t_k to t_{k+1} ($k = 0, 1, 2, \dots$) are applied in a receding horizon scheme as follows:

$$u_i(t) = u_i^*(t|t_k), \quad i = 1, \dots, m, \quad \forall t \in [t_k, t_{k+1}) \quad (8)$$

To proceed for the closed-loop stability analysis, we need the following propositions.

Proposition 1 (c.f. [16]). Consider the systems:

$$\begin{aligned} \dot{x}_a(t) &= f(x_a(t), u_1(t), \dots, u_m(t), w(t)) \\ \dot{x}_b(t) &= f(x_a(t), u_1(t), \dots, u_m(t), 0) \end{aligned} \quad (9)$$

with initial states $x_a(t_0) = x_b(t_0) \in \Omega_{\rho}$. There exists a class \mathcal{K} function $f_W(\cdot)$ such that:

$$|x_a(t) - x_b(t)| \leq f_W(t - t_0), \quad (10)$$

for all $x_a(t), x_b(t) \in \Omega_{\rho}$ and all $w(t) \in W$ with $f_W(\tau) = L_w \theta(e^{L_x \tau} - 1)/L_x$.

Proposition 1 provides an upper bound on the deviation of the state trajectory obtained using the nominal model, from the actual system state trajectory when the same control input trajectories are applied. Proposition 2 below bounds the difference between the magnitudes of the Lyapunov function of two different states in Ω_{ρ} .

Proposition 2 (c.f. [16]). Consider the Lyapunov function $V(\cdot)$ of the system of Eq. (1). There exists a quadratic function $f_V(\cdot)$ such that:

$$V(x) \leq V(\tilde{x}) + f_V(|x - \tilde{x}|) \quad (11)$$

for all $x, \tilde{x} \in \Omega_{\rho}$ with $f_V(s) = \alpha_4(\alpha_1^{-1}(\rho))s + M_v s^2$ where M_v is a positive constant.

Proposition 3 below ensures that if the nominal system controlled by $h(x)$ implemented in a sample-and-hold fashion and with open-loop state estimation starts in Ω_{ρ} , then it is ultimately bounded in $\Omega_{\rho_{\min}}$.

Proposition 3 (c.f. [16]). Consider the nominal sampled trajectory $\hat{x}(t)$ of the system of Eq. (1) in closed-loop for a controller $h(x)$, which satisfies the condition of Eq. (2), obtained by solving recursively:

$$\dot{\hat{x}}(t) = f(\hat{x}(t), h_1(\hat{x}(t_k)), \dots, h_m(\hat{x}(t_k)), 0) \quad (12)$$

where $t \in [t_k, t_{k+1})$ with $t_k = t_0 + k\Delta, k = 0, 1, \dots$. Let $\Delta, \epsilon_s > 0$ and $\rho > \rho_s > 0$ satisfy:

$$-\alpha_3(\alpha_2^{-1}(\rho_s)) + L'_x M \Delta \leq \frac{-\epsilon_s}{\Delta} \quad (13)$$

Then, if $\hat{x}(t_0) \in \Omega_{\rho}$ and $\rho_{\min} < \rho$ where $\rho_{\min} = \max\{V(x(t + \Delta)) : V(x(t)) \leq \rho_s\}$, the following inequality holds: $V(\hat{x}(t)) \leq V(\hat{x}(t_k)), \forall t \in [t_k, t_{k+1})$ and $V(\hat{x}(t_k)) \leq \max\{V(\hat{x}(t_0)) - k\epsilon_s, \rho_{\min}\}$.

Theorem 1 below provides sufficient conditions under which the LEMPC of Eq. (7) guarantees that the state of the closed-loop system is always bounded in Ω_{ρ} and is ultimately bounded in a small region containing the origin.

Theorem 1. Consider the system of Eq. (1) in closed-loop under the distributed LEMPC design of Eq. (7) based on a controller $h(x)$ that satisfies the conditions of Eq. (2). Let $\epsilon_w > 0, \Delta > 0, \rho > \tilde{\rho} > 0$ and $\rho > \rho_s > 0$ satisfy:

$$\tilde{\rho} \leq \rho - f_V(f_W(\Delta)) \quad (14)$$

and

$$-\alpha_3(\alpha_2^{-1}(\rho_s)) + L'_x M \Delta + L'_w \theta \leq \frac{-\epsilon_w}{\Delta} \quad (15)$$

If $x(t_0) \in \Omega_{\rho}, \rho_s \leq \tilde{\rho}, \rho_{\min} \leq \rho$ and $N \geq 1$, then the state $x(t)$ of the closed-loop system is always bounded in Ω_{ρ} and is ultimately bounded in $\Omega_{\rho_{\min}}$ with ρ_{\min} defined in Proposition 3.

Proof: The proof consists of three parts. We first prove that the optimization problem of Eq. (7) is feasible for all states $x \in \Omega_{\rho}$. Subsequently, we prove that, in the first operation mode, under the LEMPC design of Eq. (7), the closed-loop state of the system of Eq. (1) is always bounded in Ω_{ρ} . Finally, we prove that, in the second operation mode, under the LEMPC of Eq. (7), the closed-loop state of the system of Eq. (1) is ultimately bounded in ρ_{\min} .

Part 1: When $x(t)$ is maintained in Ω_{ρ} (which will be proved in Part 2), the feasibility of the distributed EMPC (DEMPC) of Eq. (7) follows because input trajectory $u_j(t), j = 1, \dots, m$, such that $u_j(t) = h_j(x(t_{k+q})), \forall t \in [t_{k+q}, t_{k+q+1})$ with $q = 0, \dots, N - 1$ is a feasible solution to the optimization problem of Eq. (7) since such trajectory satisfied the input constraint of Eq. (7e) and the Lyapunov-based constraints of Eqs. (7g) and (7h). This is guaranteed by the closed-loop stability property of the Lyapunov-based controller $h(x)$; the reader may refer to [19] for more detailed discussion on the stability property of the Lyapunov-based controller $h(x)$.

Part 2: We assume that the LEMPC of Eq. (7) operates in the first operation mode. We prove that if $x(t_k) \in \Omega_{\tilde{\rho}}$, then $x(t_{k+1}) \in \Omega_{\rho}$; and if $x(t_k) \in \Omega_{\rho}/\Omega_{\tilde{\rho}}$, then $V(x(t_{k+1})) < V(x(t_k))$ and in finite steps, the state converges to $\Omega_{\tilde{\rho}}$ (i.e., $x(t_{k+j}) \in \Omega_{\tilde{\rho}}$ where j is a finite positive integer).

When $x(t_k) \in \Omega_{\tilde{\rho}}$, from the constraint of Eq. (7g), we obtain that $\tilde{x}^1(t_{k+1}) \in \Omega_{\tilde{\rho}}$. By Propositions 1 and 2, we obtain the following inequality:

$$V(x(t_{k+1})) \leq V(\tilde{x}^1(t_{k+1})) + f_V(f_W(\Delta)) \quad (16)$$

Note that LEMPC 1 has access to all of the optimal input trajectories of the other distributed controllers evaluated before it. Since $V(\tilde{x}^1(t_{k+1})) \leq \tilde{\rho}$, if the condition of Eq. (14) is satisfied, we can conclude that:

$$x(t_{k+1}) \in \Omega_{\rho}$$

When $x(t_k) \in \Omega_{\rho}/\Omega_{\tilde{\rho}}$, from the constraint of Eq. (7h) and the condition of Eq. (2), we can obtain:

$$\begin{aligned} & \frac{\partial V(x(t_k))}{\partial x} f(x(t_k), u_1^*(t_k|t_k), \dots, u_m^*(t_k|t_k), 0) \\ & \leq \frac{\partial V(x(t_k))}{\partial x} f(x(t_k), h_1(x(t_k)), u_2^*(t_k|t_k), \dots, u_m^*(t_k|t_k), 0) \\ & \leq \dots \\ & \leq \frac{\partial V(x(t_k))}{\partial x} f(x(t_k), h_1(x(t_k)), \dots, h_m(x(t_k)), 0) \\ & \leq -\alpha_3(|x(t_k)|) \end{aligned} \quad (17)$$

The time derivative of the Lyapunov function along the actual system state $x(t)$ for $t \in [t_k, t_{k+1})$ can be written as follows:

$$\dot{V}(x(t)) = \frac{\partial V(x(t))}{\partial x} f(x(t), u_1^*(t_k|t_k), \dots, u_m^*(t_k|t_k), w(t)) \quad (18)$$

Adding and subtracting $(\partial V(x(t_k)))/(\partial x) f(x(t), u_1^*(t_k|t_k), \dots, u_m^*(t_k|t_k), 0)$ to/from the above equation and accounting for Eq. (17), we have:

$$\begin{aligned} \dot{V}(x(t)) & \leq -\alpha_3(|x(t_k)|) + \frac{\partial V(x(t))}{\partial x} f(x(t), u_1^*(t_k|t_k), \dots, u_m^*(t_k|t_k), w(t)) \\ & \quad - \frac{\partial V(x(t_k))}{\partial x} f(x(t), u_1^*(t_k|t_k), \dots, u_m^*(t_k|t_k), 0) \end{aligned} \quad (19)$$

Due to the fact that the disturbance is bounded (i.e., $|w| \leq \theta$) and the Lipschitz properties of Eq. (4), we can write:

$$\dot{V}(x(t)) \leq -\alpha_3(\alpha_2^{-1}(\rho_s)) + L'_x|x(t) - x(t_k)| + L_w\theta \quad (20)$$

Taking into account Eq. (3) and the continuity of $x(t)$, the following bound can be written for all $\tau \in [t_k, t_{k+1})$

$$|x(\tau) - x(t_k)| \leq M\Delta \quad (21)$$

Since $x(t_k) \in \Omega_{\rho}/\Omega_{\tilde{\rho}}$, it can be concluded that $x(t_k) \in \Omega_{\rho}/\Omega_{\rho_s}$. Thus, we can write for $t \in [t_k, t_{k+1})$:

$$\dot{V}(x(t)) \leq -\alpha_3(\alpha_2^{-1}(\rho_s)) + L'_x M\Delta + L_w\theta \quad (22)$$

If the condition of Eq. (15) is satisfied, then there exists $\epsilon_w > 0$ such that the following inequality holds for $x(t_k) \in \Omega_{\rho}/\Omega_{\tilde{\rho}}$:

$$\dot{V}(x(t)) \leq \frac{-\epsilon_w}{\Delta}, \quad \forall t = [t_k, t_{k+1})$$

Integrating this bound on $t \in [t_k, t_{k+1})$, we obtain that:

$$\begin{aligned} V(x(t_{k+1})) & \leq V(x(t_k)) - \epsilon_w \\ V(x(t)) & \leq V(x(t_k)), \quad \forall t \in [t_k, t_{k+1}) \end{aligned} \quad (23)$$

for all $x(t_k) \in \Omega_{\rho}/\Omega_{\tilde{\rho}}$. Using Eq. (23) recursively, it is proved that, if $x(t_k) \in \Omega_{\rho}/\Omega_{\tilde{\rho}}$, the state converges to $\Omega_{\tilde{\rho}}$ in a finite number of sampling times without leaving Ω_{ρ} .

Part 3: We assume that the DEMPC of Eq. (7) operates in the second operation mode. We prove that if $x(t_k) \in \Omega_{\rho}$, then $V(x(t_{k+1})) \leq V(x(t_k))$ and the system state is ultimately bounded in an invariant set $\Omega_{\rho_{\min}}$. Following the similar steps as in Part 2, we can derive that the inequality of Eq. (23) hold for all $x(t_k) \in \Omega_{\rho}/\Omega_{\rho_s}$. Using this result recursively, it is proved that, if $x(t_k) \in \Omega_{\rho}/\Omega_{\rho_s}$, the state converges to Ω_{ρ_s} in a finite number of sampling times without leaving Ω_{ρ} . Once the state converges to $\Omega_{\rho_s} \subseteq \Omega_{\rho_{\min}}$, it remains

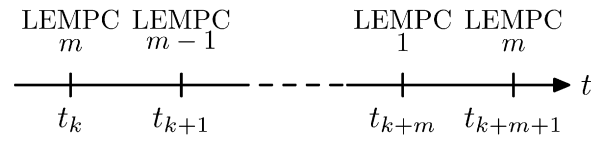


Fig. 4. Distributed controller evaluation sequence.

inside $\Omega_{\rho_{\min}}$ for all times. This statement holds because of the definition of ρ_{\min} . This proves that the closed-loop system under the LEMPC of Eq. (7) is ultimately bounded in $\Omega_{\rho_{\min}}$.

4.2. Implementation strategy II

In the implementation strategy introduced in the previous subsection, the evaluation time of the distributed LEMPC at a sampling time is the summation of the evaluation times of all the distributed controllers; this is because at each sampling time all distributed controllers are evaluated in a sequential fashion. However, for applications in which a small sampling time needs to be used and fast controller evaluation is required, we may distribute the evaluation of the distributed controllers into multiple sampling periods. In this implementation strategy, the distributed controllers are evaluated in sequence but over several sampling times and only one controller is evaluated at each sampling time. Fig. 4 shows a possible evaluation sequence of the distributed controllers in this implementation strategy. In Fig. 4, at t_k , LEMPC m is evaluated and it sends the input trajectories of u_m to LEMPC $m-1$; at t_{k+1} , LEMPC $m-1$ is evaluated and it sends u_m and u_{m-1} to LEMPC $m-2$; from time t_{k+2} to t_{k+m} , LEMPC $m-2$ to LEMPC 1 are evaluated in sequence and one complete distributed control system evaluation cycle is carried out. Another controller evaluation cycle starts at t_{k+m+1} with the evaluation of LEMPC m again. In order to guarantee the closed-loop stability of this implementation strategy, the design of the distributed LEMPC of Eq. (7) needs to be modified to account for the multiple sampling time evaluation cycle. We note that both implementation strategy I and implementation strategy II can be executed using parallel computing.

Remark 1. Referring to the choice of the Lyapunov function in the context of a specific chemical process application, we note the following: first, an economically-optimal equilibrium point is computed as the solution of the steady-state optimization problem of Eq. (6). This equilibrium point is then used to construct a Lyapunov function for the process expressed in terms of state variable deviations from this equilibrium point (in most applications, quadratic Lyapunov functions can be used; please see application example in Section 5). Subsequently, this Lyapunov function is used for the design of a state feedback controller $h(x)$ and the computation of the set of initial conditions starting from where closed-loop stability (i.e., convergence to a small neighborhood of the economically-optimal equilibrium point) is guaranteed. This set is typically a level set, Ω_{ρ} , of the Lyapunov function V embedded within the set where the time derivative of V along the trajectories of the nonlinear closed-loop system with $h(x)$ is negative. Therefore, the construction of Ω_{ρ} accounts explicitly for the process nonlinearity and it is not a local (i.e., based on the linearization) stability region. Referring to the economic MPC, we note that no assumption is made that the optimization problem at sampling time t_k with $x(t_k) \in \Omega_{\rho}$ has a unique solution. Due to the incorporation of the Lyapunov-based constraint of Eq. (7h), for any $x(t_k) \in \Omega_{\rho}$, the economic MPC problem has a solution; the one defined by $h(x)$. Therefore, the purpose of the optimization problem is to compute control actions over the prediction horizon that optimize the cost of Eq. (7) further, yet they satisfy the Lyapunov-based constraint of Eq. (7h). Given the constraint that $x(t)$, $t \in [t_k, t_{k+N}]$, stays in Ω_{ρ} , the

Table 4

Manipulated input constraints for all controllers.

$ \tilde{u}_1 \leq 3.5 \times 10^5$ [J/s]	$ \tilde{u}_2 \leq 3.5 \times 10^5$ [J/s]
$ \tilde{u}_3 \leq 7 \times 10^5$ [J/s]	$ \tilde{u}_4 \leq 10 \times 10^5$ [J/s]
$ \tilde{u}_5 \leq 3 \times 10^5$ [J/s]	$ \tilde{u}_i \leq 1.7394 \times 10^{-4}$ [m ³ /s] ($i = 6, 7, 8$)

economic MPC optimization problem can be solved either locally or globally (with respect to its optimum) within Ω_ρ , depending on the type of optimal solution that is required to be found. Note that during mode 1 operation under the economic MPC of Eq. (7), the Lyapunov constraint is not used to steer the closed-loop system state to the economically-optimal equilibrium point used in the construction of the Lyapunov function but it is simply used to constrain the closed-loop state within a certain operating set (typically Ω_ρ) where feasibility of the economic MPC optimization problem is guaranteed. As a consequence, there is no need to impose explicit constraints that limit the discrepancy between $h(x)$ and the economic MPC-based control action in the centralized LEMPC case. Finally, due to the use of a finite sampling time, asymptotic stability of the final equilibrium point can not be studied instead practical stability (i.e., ultimate boundedness of the state in a small ball containing the desired steady-state) is studied.

5. Application to nonlinear chemical process network

In this section, we apply the two economic MPC architectures to the process; that is: the centralized Lyapunov-based economic MPC and the sequential distributed Lyapunov-based economic MPC. The objective of all controllers is to drive the system from the stable steady-state defined in Table 1 to the economically optimal steady-state. We will also compare the performance of the economic MPC and DMPC with the performance of a conventional centralized MPC utilizing a quadratic cost function.

5.1. Preliminaries

We begin with some preliminaries that will be used in the formulations of the various MPC designs. All MPCs utilize the following Lyapunov function $V(x) = (x - x^s)^T P (x - x^s)$ with P being the same matrix as in Section 3.2. We assume that the state x of the system is sampled synchronously and the time instants at which we have state measurements are indicated by the time sequence $t_{k \geq 0}$ with $t_k = t_0 + k\Delta$, $k = 0, 1, \dots$ where t_0 is the initial time and Δ is the sampling time. The manipulated input in this control problem is defined below with respect to the optimal steady-state input values:

$$\tilde{U} = [\tilde{u}_1 \dots \tilde{u}_8] = [u_1 - u_1^s \dots u_8 - u_8^s]$$

The constraints that all MPC controllers have to satisfy are listed in Table 4. It is important to note that even though the input constraints have been modified accordingly, the set U still satisfies the constraints in Table 2.

The process model in [16] belongs to the following class of nonlinear systems (which is included in the broad class of nonlinear systems of Eq. (1)):

$$\dot{x}(t) = f(x) + \sum_{i=1}^8 g_i(x) \tilde{u}_i$$

where the state x is the deviation of the states variables from the economically-optimal steady-state. For the control of the process, the input $\tilde{u}_1, \tilde{u}_2, \tilde{u}_3, \tilde{u}_4$ and \tilde{u}_5 are necessary to keep the stability of the closed-loop system, while \tilde{u}_6, \tilde{u}_7 and \tilde{u}_8 can be used as extra inputs to improve the closed-loop performance. The design of the

Lyapunov-based controller $h_i(x)$, $i = 1, \dots, 5$ is based on Sontag's formula [24]:

$$h_i(x) = \begin{cases} -\frac{L_f V + \sqrt{(L_f V)^2 + (L_{g_i} V)^4}}{(L_{g_i} V)^2} L_{g_i} V & \text{if } L_{g_i} V \neq 0 \\ 0 & \text{if } L_{g_i} V = 0 \end{cases}$$

where $i = 1, \dots, 5$, $L_f V = (\partial V / \partial x) f(x)$ and $L_{g_i} V = (\partial V / \partial x) g_i(x)$ denote the Lie derivatives of the scalar function V with respect to the vector fields f and g_i , respectively. The controllers $h_6(x)$, $h_7(x)$ and $h_8(x)$ are chosen to be 0.

For comparison purposes, we consider the following objective function of the conventional centralized MPC:

$$J = \sum_{i=0}^{N\Delta} [x(t_i)^T Q_c x(t_i) + \sum_{j=1}^8 u_j(t_i)^T R_{c_j} u_j(t_i)] \quad (24)$$

the weighting matrices are chosen to be $Q_c = \text{diag}([1 \ 1 \ 1 \ 1 \ 10^3 \ 1 \ 1 \ 1 \ 10^3 \ 10 \ 10 \ 10 \ 10 \ 10^4 \ 1 \ 1 \ 1 \ 1 \ 10^3 \ 1 \ 1 \ 1 \ 10^3])$, and $R_{c_j} = \text{diag}([10^{-8} \ 10^{-8} \ 10^{-8} \ 10^{-8} \ 10^{-8} \ 1 \ 1 \ 1])$.

Remark 2. Referring to the computation of $V(x)$, we note that the computation of \dot{V} was carried out on the basis of the nonlinear vector fields of the process dynamic model and not on the basis of any type of linearization. Furthermore, the matrix P was computed via simulations to maximize: (a) the region where \dot{V} of the closed-loop system under the Lyapunov-based controller is negative and (b) the corresponding closed-loop system stability region Ω_ρ . We also note that the terms in P were scaled based on the different magnitudes of the state variables.

Remark 3. Referring to the switching time t' , we note that t' depends on the amount of time that we want to spend to economically optimize the closed-loop system while keeping the closed-loop system state in an invariant set.

5.2. Centralized LEMPC

The centralized Lyapunov-based economic MPC design follows the formulation of our previous work [8] with minor modifications (appropriate for the chemical process example in this work) as follows:

$$\tilde{u}_j^*(t_k) = \max_{u_j \in S(\Delta)} \int_{t_k}^{t_{k+N}} L(\tilde{x}(\tau), \tilde{u}_j(\tau)) d\tau \quad (25a)$$

$$\text{s.t. } \dot{\tilde{x}}(t) = f(\tilde{x}(t)) + \sum_{i=1}^8 g_i(\tilde{x}(t)) \tilde{u}_i(t) \quad (25b)$$

$$\forall t \in [t_k, t_{k+1}), \quad k = 0, \dots, N-1 \\ \tilde{u}_j(t) \in U_j \quad (25c)$$

$$\tilde{x}(t_k) = x(t_k) \quad (25d)$$

$$\sum_{i=2,4,6} F_i = F^{\max} \quad (25e)$$

Mode one:

$$\tilde{x}(t_k) \in X \quad (25f)$$

$$V(\tilde{x}(t_k)) \leq \tilde{\rho}_e \quad (25g)$$

Mode two:

$$\frac{\partial V(\tilde{x}(t_k))}{\partial x} g_j(\tilde{x}(t_k)) u_j(t_k) \leq \inf_{t \in [t_{k-1}, t_k]} \frac{\partial V(\tilde{x}(t))}{\partial x} g_j(\tilde{x}(t)) h_j(\tilde{x}(t)) \quad (25h)$$

where \tilde{x} is the predicted closed-loop system state, $S(\Delta)$ is the family of piecewise constant function with period Δ and $t_{k+N} = t_k + N\Delta$. The

economic measure L of Eq. (25) has the same set up as in Section 3.2 Eq. (5) and Eq. (25e) imposes the quantity constraint of reactant B, from which F_{\max} has the same value as in Section 3.2.

At mode one operation, Eq. (25f) of the formulation ensures that the state variable $\tilde{x}(t_k)$ that has been obtained by applying the solution $\tilde{u}_j^*(t_k)$ is bounded. It is important to distinguish the difference between the constraints of Eq. (6d) and Eq. (25f). Since steady-state optimization focuses on a steady-state solution, Eq. (6d) merely states that the solution has to be bounded; however, the economic MPC, which is a finite-horizon dynamic optimization problem, has to enforce a more aggressive constraint on the closed-loop state trajectory, where the state variables at the end of each sampling time have to be bounded. With respect to the constraint $x(t_k) \in X$, we require that the state variables $x(t_k)$ remain within $\pm 6\%$ of their initial steady-state values for all times; note that the economically optimal steady-state is within X . The level set ρ_e is chosen to be 1.45×10^6 . At mode two operation, the constraint of Eq. (25h) is a tighter version of the Lyapunov-based constraint in [8], and it is used to ensure that the closed-loop system state converges sufficiently close to the economically optimal steady-state.

5.3. Sequential distributed LEMPC

In this section, we design a sequential distributed LEMPC architecture for the benzene process. Specifically, the first distributed model predictive controller (DMPC 1) obtains the optimal values of \tilde{u}_4 and \tilde{u}_5 , the second distributed controller (DMPC 2) is designed to obtain the optimal values of \tilde{u}_1 , \tilde{u}_2 and \tilde{u}_3 , while the third distributed controller (DMPC 3) is designed to obtain the optimal values of \tilde{u}_6 , \tilde{u}_7 and \tilde{u}_8 . Specifically, DMPC j ($j=1, 2, 3$) can be formulated as follows:

$$u_{s,j}^*(t_k) = \max_{u_{s,j} \in S(\Delta)} \int_{t_k}^{t_k+N} L(\tilde{x}(\tau), \tilde{u}_{s,j}(\tau)) d\tau \quad (26a)$$

$$\text{s.t. } \dot{\tilde{x}}(t) = f(\tilde{x}(t)) + \sum_{i=1}^8 g_i(\tilde{x}(t)) \tilde{u}_{s,i}(t) \quad (26b)$$

$$\forall t \in [t_k, t_{k+1}), \quad k = 0, \dots, N-1 \quad (26c)$$

$$\tilde{u}_{s,i}(t_k) = u_{s,i}^*(t_k), \quad i = 1, \dots, j-1 \quad (26d)$$

$$\tilde{u}_{s,i}(t_k) = h_i(\tilde{x}(t_k)), \quad i = j, \dots, m \quad (26e)$$

$$\tilde{u}_{s,j}(t) \in U_j \quad (26f)$$

$$\tilde{x}(0) = x(t_k) \quad (26g)$$

$$\sum_{i=\{2,4,6\}} F_i = F^{\max} \quad (26g)$$

Mode one:

$$\tilde{x}(t_k) \in X_s \quad (26h)$$

$$V(\tilde{x}(t_k)) \leq \tilde{\rho}_e \quad (26i)$$

Mode two:

$$\frac{\partial V(\tilde{x}(t_k))}{\partial x} g_j(\tilde{x}(t_k)) u_j(t_k) \leq \frac{\partial V(x(t_k))}{\partial x} g_j(\tilde{x}(t_k)) h_j(\tilde{x}(t_k)) \quad (26j)$$

where the economic measure L has the same form as in Section 3.2 Eq. (5) and F^{\max} and $\tilde{\rho}_e$ have the same values as in Section 5.2.

Since each DMPC controller is designed to obtain a subset of the manipulated inputs, the state constraint enforced in the centralized Lyapunov-based economic MPC design may not be satisfied in each DMPC calculation, and thus, a relaxed version of this constraint is used where we require that the state variables $x(t_k)$ remain within $\pm 7\%$ of their initial steady-state values for all times in all DMPC calculations. Thus, appropriate bounds on the initial state condition needs to be enforced (close enough to the desired steady-state).

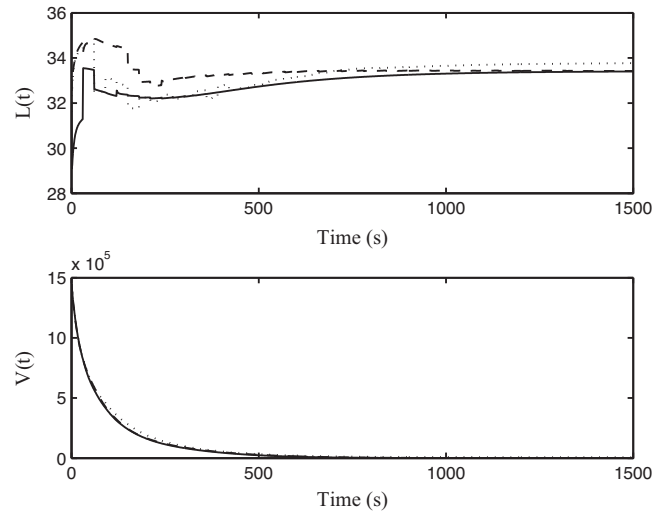


Fig. 5. Trajectories of the economic measure and of the Lyapunov function using the centralized LMPC with conventional quadratic cost of Eq. (24) (solid line), the centralized LEMPC (dashed line) at mode two, and the DLEMPC (dotted line) at mode two. The prediction horizon $N=3$.

5.4. Closed-loop simulation results

The simulations were performed in a JAVA platform by a Core2 Quad Q6600 computer. The simulation time for each run is 3000 s. Three different simulation cases are studied here in order to evaluate the properties of the proposed controller designs. The first case studies the closed-loop system performance by the centralized LEMPC and by the DLEMPC both operating at mode two. The second case studies the closed-loop system performance by the same controllers but operating at mode one. In the last case, we study the closed-loop system performance by the same controllers operating at mode one first and then at mode two. We will compare the closed-loop system performance of the economic MPC to the performance of the conventional centralized Lyapunov-based MPC (LMPC) which uses the conventional quadratic cost function of Eq. (24).

All simulation studies apply the same prediction horizon, which is $N=3$. Only the first piece from the computed optimal input trajectory of the optimization problems is implemented in each sampling time following a receding horizon scheme. The sampling time of the optimization problems is $\Delta=30$ s, and as a result, the total number of sampling times along one simulation is one hundred. All state measurements are available to the MPC controllers at each sampling time.

The numerical method that is used to integrate the process model is explicit Euler with a fixed time step equal to 0.5 s. Again, as in the case of steady-state optimization, the optimization problems of each MPC scheme are solved using the open source interior point optimizer Ipopt. The Hessian is approximated by Quasi-Newton's method. Regarding the termination criteria and the maximum number of iterations, the values used by all simulations are 10^{-3} and 200, respectively.

The results of case one are shown in Figs. 5 and 6. It is important to note that even though the conventional centralized MPC does not use the economic measure as its objective function, we recalculate its performance from an economic perspective based on Eq. (25a) and include it in the figures. The Lyapunov function in Fig. 5 clearly indicates that both economic MPC schemes stabilize the process asymptotically to the optimal steady state. Specifically, the centralized LEMPC drives the system to the optimal steady-state, and in terms of accumulated economic measure, it performs better than the conventional MPC controller by 1.5% up to 1000 s of simulation

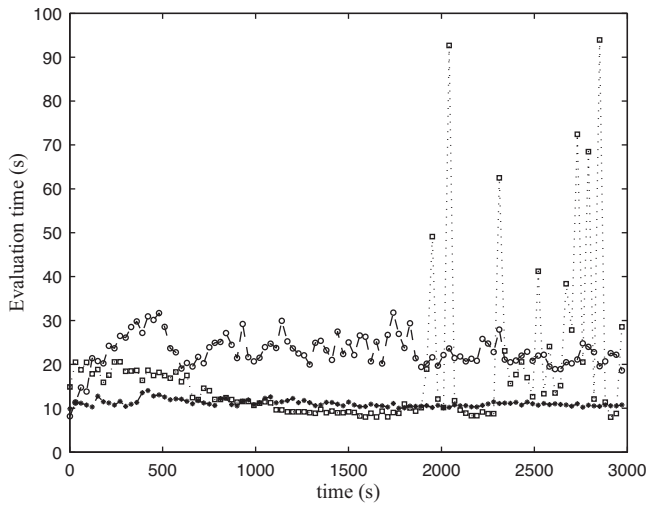


Fig. 6. The total evaluation time needed for evaluation of each MPC method. Centralized LMPC with conventional quadratic cost of Eq. (24) (dotted line with squares), the centralized LEMPC (dashed line with circles) at mode two, and the DLEMPC (solid line with asterisks) at mode two. The prediction horizon $N=3$.

time. In contrast, there exists an offset of the economic measure of the DLEMPC, and that is in coincidence with the fact that the value of its Lyapunov function converges to a non-zero positive number at the end. We note here that even though all simulations reported in Figs. 5, 7 and 9 have been carried out using a total simulation time of 3000 s, in order to better show the initial transient behavior in Figs. 5 and 9, we report the results up to 1500 s where the trajectories of all simulations have reached steady-state.

With respect to the centralized LEMPC, we notice that the offset is caused primarily by the structure of the DLEMPC. While each DMPC controller accomplishes each mission successfully according to its formulation, the overall closed-loop cost does not converge to the one of the centralized LEMPC.

With respect to the evaluation time of the different controllers at each sampling time, the DLEMPC outperforms the centralized LEMPC by more than 50% in average and even the centralized MPC at the beginning. It is important to note that the total evaluation time required for the DLEMPC in one sampling time is the sum of the

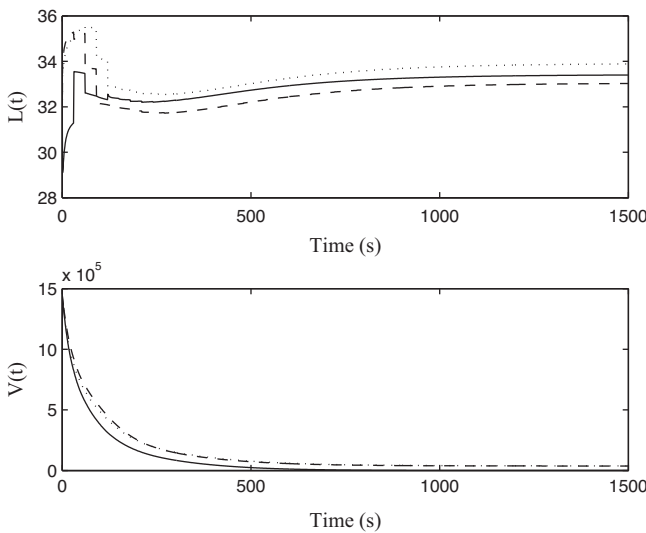


Fig. 7. Trajectories of the economic measure and of the Lyapunov function using the centralized LMPC with conventional quadratic cost of Eq. (24) (solid line), the centralized LEMPC (dashed line) at mode one, and the DLEMPC (dotted line) at mode one. The prediction horizon $N=3$, and the level set $\tilde{\rho}_e = 1.45 \times 10^6$.

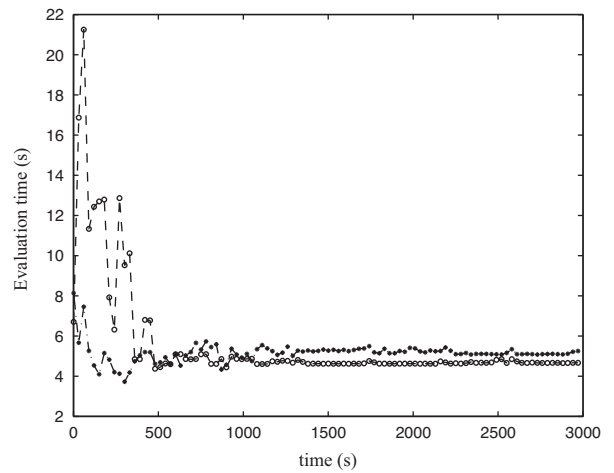


Fig. 8. The total evaluation time needed for each evaluation of centralized LMPC (dashed line with circles) at mode one and DLEMPC (solid line with asterisks) at mode one. The prediction horizon $N=3$.

evaluation times of all the DMPC controllers. We also observe that the evaluation time of centralized LMPC overshoots at few sampling times after $t = 1800$ s. This increase in the controller evaluation time is due to a significant sampling time which allows for deviation of the closed-loop trajectories from the steady-state, as well as the effort of the controller to satisfy the Lyapunov constraint in the first move and the non-convexity of the optimization problem.

The results of case two are shown in Figs. 7 and 8. The Lyapunov function of Fig. 7 indicates that starting from $\tilde{\rho}_e = 1.45 \times 10^6$, both control schemes are not able to stabilize the closed-loop system to the economically optimal steady-state but converge to a region with their V values approximately equal to $\tilde{\rho} = 1 \times 10^5$. This result is expected since as we have mentioned in Section 3.2 the economically optimal operating steady-state is an unstable steady state. Looking at the economic measure, even though both control schemes have similar value of the Lyapunov function at the end, the DLEMPC has a higher economic measure overall compared with the one of the centralized economic MPC. The reason is due to the different state constraints imposed in each of their problem formulations. Finally, comparing the evaluation time of the different MPC schemes at mode one, we see that, as expected, the DLEMPC outperforms the other schemes at the first 500 s. The average control action evaluation times for the different cases are summarized in Table 5.

The last two figures (Figs. 9 and 10) belong to the study of case three, for which we want to demonstrate that the controllers can switch their operating mode between mode one and mode two under either the centralized LEMPC or the DLEMPC; the switching choice, depends on the control objective, e.g., fast computational time or offset elimination. Finally, it is worthwhile to discuss few benefits of using economic MPC instead of conventional MPC based on the results of this study. First, the centralized LEMPC is characterized by an improved coupling between the different layers of a plant-wide process control system, in particular, the economic

Table 5
Average control action evaluation time.

		Average control action evaluation time	
LEMPC	Mode 1	22.91 s	5.58 s
	Mode 2		
DLEMPC	Mode 1	11.10 s	5.16 s
	Mode 2		
Centralized LMPC		17.49 s	

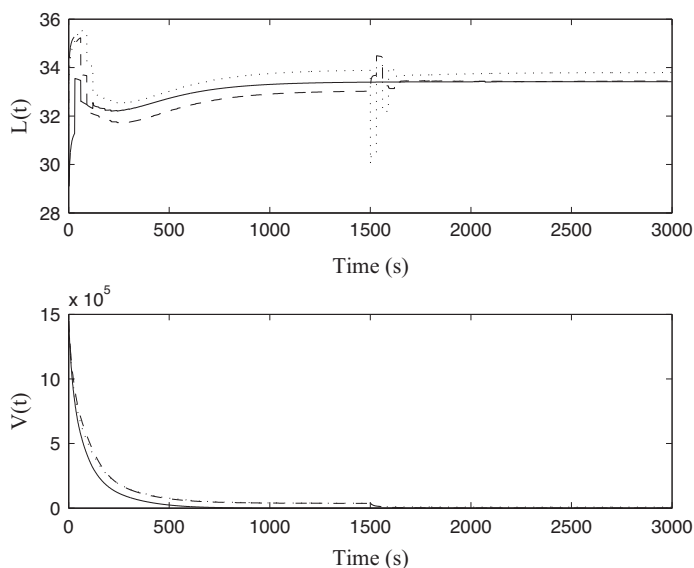


Fig. 9. Trajectories of the economic measure and of the Lyapunov function by centralized LMPC with conventional quadratic cost of Eq. (24) (solid line), the centralized LMPC (dashed line), and the DLEMPC (dotted line). The last two operate at mode one up to $t = 1500$ s and subsequently at mode two. The prediction horizon $N = 3$, and the level set $\hat{\rho}_e = 1.45 \times 10^6$.

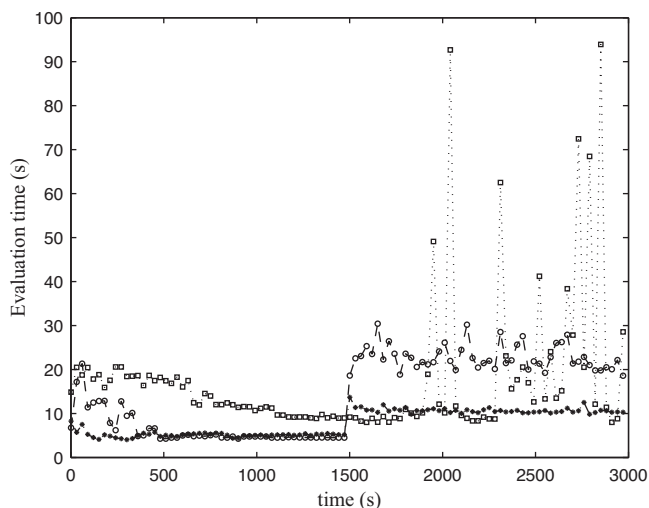


Fig. 10. The total evaluation time needed for each evaluation of MPC method corresponding to Fig. 9. Centralized LMPC with conventional quadratic cost of Eq. (24) (dotted line with squares), the centralized LMPC (dashed line with circles), and DLEMPC (solid line with asterisks). The prediction horizon $N = 3$.

optimization and process control layer. In terms of performance, the economic MPC is able to drive the system to the set-point for higher profit return with comparable computational time. Another benefit of applying economic MPC is the ease of tuning. It is a difficult task to assign a reasonable value to the parameters of conventional MPC with quadratic cost since very often they do not have any physical meaning. On the other hand, all parameters of economic MPC have specific economic meaning, and thus, their tuning is more intuitive.

6. Conclusions

In this work, we carried out an application of centralized LEMPC and sequential distributed LEMPC architectures to a catalytic alkylation of benzene process network which consists of four continuous stirred tank reactors and a flash separator. In the

sequential distributed LEMPC design, three separate Lyapunov-based model predictive controllers were designed to control the process in a sequential coordinated fashion. The closed-loop stability properties of the sequential distributed LEMPC design were rigorously analyzed and sufficient conditions for closed-loop stability were established. Simulations were carried out to compare the proposed economic MPC architectures with a centralized LMPC which uses a quadratic cost function that includes penalty on the deviation of the states and inputs from their economically optimal steady-state values, from computational time and closed-loop performance points of view.

Acknowledgement

Financial support from the National Science Foundation is gratefully acknowledged.

References

- [1] T. Backx, O. Bosgra, W. Marquardt, Integration of model predictive control and optimization of processes: enabling technology for market driven process operation, in: Proceedings of the IFAC Symposium on Advanced Control of Chemical Processes, Pisa, Italy, 2000, pp. 249–260.
- [2] E. Camponogara, D. Jia, B.H. Krogh, S. Talukdar, Distributed model predictive control, IEEE Control Systems Magazine 22 (2002) 44–52.
- [3] P.D. Christofides, N.H. El-Farra, Control of Nonlinear and Hybrid Process Systems: Designs for Uncertainty, Constraints and Time-delays, Springer-Verlag, Berlin, Germany, 2005.
- [4] P.D. Christofides, J. Liu, D. Muñoz de la Peña, Networked and Distributed Predictive Control: Methods and Nonlinear Process Network Applications, Springer-Verlag, London, England, 2011.
- [5] M. Diehl, R. Amrit, J.B. Rawlings, A Lyapunov function for economic optimizing model predictive control, IEEE Transactions on Automatic Control 56 (2011) 703–707.
- [6] H. Ganji, J.S. Ahari, A. Farshi, M. Kakavand, Modelling and simulation of benzene alkylation process reactors for production of ethylbenzene, Petroleum and Coal 46 (2004) 55–63.
- [7] C.E. García, D.M. Prett, M. Morari, Model predictive control: theory and practice—a survey, Automatica 25 (1989) 335–348.
- [8] M. Heidarinejad, J. Liu, P.D. Christofides, Economic model predictive control of nonlinear process systems using Lyapunov techniques, AIChE Journal 58 (2012) 855–870.
- [9] R. Huang, E. Harinath, L.T. Biegler, Lyapunov stability of economically-oriented NMPC for cyclic processes, Journal of Process Control 21 (2011) 501–509.
- [10] J.V. Kadam, W. Marquardt, Integration of economical optimization and control for intentionally transient process operation, in: R. Findeisen, F. Allgöwer, L.T. Biegler (Eds.), Assessment and Future Directions of Nonlinear Model Predictive Control, LNCS, vol. 358, 2007, pp. 419–434.
- [11] P. Kokotovic, M. Arcak, Constructive nonlinear control: a historical perspective, Automatica 37 (2001) 637–662.
- [12] W.J. Lee, Ethylbenzene dehydrogenation into styrene: kinetic modeling and reactor simulation, PhD thesis, Texas A&M University, College Station, TX, USA, 2005.
- [13] Y. Lin, E.D. Sontag, A universal formula for stabilization with bounded controls, Systems and Control Letters 16 (1991) 393–397.
- [14] Y. Lin, E.D. Sontag, Y. Wang, A smooth converse Lyapunov theorem for robust stability, SIAM Journal on Control and Optimization 34 (1996) 124–160.
- [15] J. Liu, D. Muñoz de la Peña, P.D. Christofides, Distributed model predictive control of nonlinear process systems, AIChE Journal 55 (2009) 1171–1184.
- [16] J. Liu, X. Chen, D. Muñoz de la Peña, P.D. Christofides, Sequential and iterative architectures for distributed model predictive control of nonlinear process systems, AIChE Journal 56 (2010) 2137–2149.
- [17] T.E. Marlin, A.N. Hrymak, Real-time operations optimization of continuous processes, AIChE Symposium Series on CPC V (1997) 156–164.
- [18] D.Q. Mayne, J.B. Rawlings, C.V. Rao, P.O.M. Scokaert, Constrained model predictive control: stability and optimality, Automatica 36 (2000) 789–814.
- [19] D. Muñoz de la Peña, P.D. Christofides, Lyapunov-based model predictive control of nonlinear systems subject to data losses, IEEE Transactions on Automatic Control 53 (9) (2008) 2076–2089.
- [20] C. Perego, P. Ingallina, Combining alkylation and transalkylation for alkylaromatic production, Green Chemistry 6 (2004) 274–279.
- [21] J.B. Rawlings, R. Amrit, Optimizing process economic performance using model predictive control, in: L. Magni, D.M. Raimondo, F. Allgöwer (Eds.), Nonlinear Model Predictive Control, Lecture Notes in Control and Information Science Series, vol. 384, Springer, Berlin, 2009, pp. 119–138.
- [22] J.B. Rawlings, B.T. Stewart, Coordinating multiple optimization-based controllers: new opportunities and challenges, Journal of Process Control 18 (2008) 839–845.

- [23] R. Scattolini, Architectures for distributed and hierarchical model predictive control—a review, *Journal of Process Control* 19 (2009) 723–731.
- [24] E. Sontag, A 'universal' construction of Artstein's theorem on nonlinear stabilization, *Systems and Control Letters* 13 (1989) 117–123.
- [25] B. Woodle, Ethylbenzene, *Petrochemicals and Petrochemical Processing*, vol. I, Taylor & Francis Group, New York, 2006, pp. 929–941 (Chapter).
- [26] H. You, W. Long, Y. Pan, The mechanism and kinetics for the alkylation of benzene with ethylene, *Petroleum Science and Technology* 24 (2006) 1079–1088.