Chapter 1
Introduction

1.1 Motivation

Optimal operation and control of dynamic systems and processes has been a subject of significant research for many years. Within the chemical process industries, operating a process for any substantial length of time at globally optimal operating conditions with respect to some meaningful economic-oriented performance criterion is almost certainly impossible. Room for process operational performance improvement will always exist.

One methodology for improving process performance while achieving operational targets and constraints is to employ the solution of optimal control problems (OCPs) on-line. In other words, control actions for the manipulated inputs of a process are computed by formulating and solving on-line a dynamic optimization problem. With the available computing power of modern computers, solving complex dynamic optimization problems, which may take the form of large-scale, nonlinear, and non-convex optimization problems, on-line is becoming an increasingly viable option. The resulting controller design may be capable of improving the closed-loop dynamic and steady-state performance relative to other controller designs.

The process performance of a chemical process typically refers to the process economics and encapsulates many objectives: profitability, efficiency, variability, capacity, sustainability, etc. As a result of continuously changing process economics, e.g., variable feedstock, changing energy prices, variable customer demand, process operation objectives and strategies need to be frequently updated to account for these changes. Traditionally, a hierarchical strategy for planning/scheduling, optimization, and control has been employed in the chemical process industries. A block diagram of the hierarchical strategy is shown in Fig. 1.1 (adapted from [1]). Although the block diagram provides an overview of the main components, it is a simplified view of modern planning/scheduling, optimization, and control systems employed in the chemical process industry in the sense that each layer may be comprised of many distributed and hierarchical computing units. The underlying design principle of the hierarchical strategy invokes time-scale separation arguments between the

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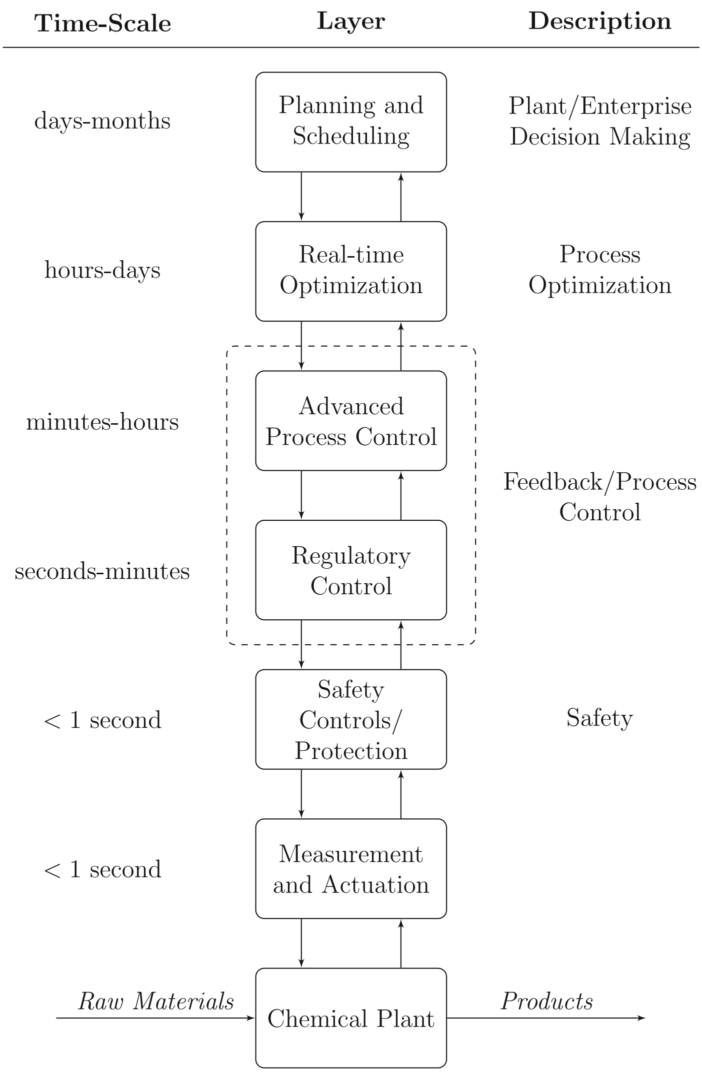

Fig. 1.1 The traditional hierarchical paradigm employed in the chemical process industries for planning/scheduling, optimization, and control of chemical plants (adapted from [1])

execution/evolution of each layer (Fig. 1.1). In the highest level of the hierarchy, enterprise-wide and/or plant-wide planning and scheduling decisions are made on the order of days-months. These decisions are made on the basis of multiple operating processes even multiple operating plants, and are out-of-scope of the present monograph.

In the next layers of the hierarchy of Fig. 1.1, economic optimization and control of chemical processes is addressed in the multi-layer hierarchical architecture, e.g., [2, 3]. The upper-layer, called real-time optimization (RTO), is responsible for process optimization. Within the RTO layer, a metric, defining the operating profit or operating cost, is optimized with respect to an up-to-date and rigorous steady-state process model to compute the optimal process steady-state. The computed steady-state is sent to the feedback process control systems, which consists of the supervisory control and regulatory control layers. The process control system steers the process to operate at the steady-state using the manipulated inputs of the process. The process control system must work to reject disturbances and ideally guide the trajectory of the process dynamics along an optimal path to the steady-state.

The advanced or supervisory process control layer of Fig. 1.1 consists of control algorithms that are used to account for process constraints, coupling of process variables and processing units, and operating performance. In the advanced process control layer, model predictive control (MPC), a control strategy based on optimal control concepts, has been widely implemented in the chemical process industry. MPC uses a dynamic model of the process in an optimization problem to predict the future evolution of the process over a finite-time horizon and to determine the optimal input trajectory with respect to a performance index. Furthermore, MPC can account for the process constraints and multi-variable interactions in the optimization problem. Thus, it has the ability to optimally control constrained multiple-input multiple-output nonlinear systems. Handling constraints and multivariate interactions are the two key advantages of MPC relative other control designs.

The standard MPC approaches are the regulating and tracking formulations that employ a quadratic performance index. Regulating MPC is used to force the process to the (economically) optimal steady-state, while tracking MPC is used to force the process to track a pre-specified reference trajectory. The quadratic performance index is a measure of the predicted squared weighted error of the states and inputs from their corresponding steady-state or target reference values. To date, there are hundreds, if not thousands, of papers on regulating/tracking MPC addressing many issues. A complete review of the MPC literature is beyond the scope of this book. For reviews and books on regulating/tracking MPC for the process industries, the interested reader is referred to [4–15].

The regulatory control layer is composed of mostly single-input single-output control loops like proportional-integral-derivative (PID) control loops that work to implement the control actions computed by the supervisory control layer; that is, it ensures that the control actuators achieve the control action requested by the MPC layer. Often, the dynamics of the regulatory control layer and control actuators are neglected in the dynamic model used in the MPC layer owing to time-scale separation arguments.

As previously mentioned, the overall control architecture of Fig. 1.1 invokes intuitive time-scale separation arguments between the various layers. For instance, RTO is executed at a rate of hours-days, while the feedback control layers compute control actions for the process at a rate of seconds-minutes-hours [1]. Though this paradigm has been successful, we are witnessing the growing need for dynamic market-driven operations which include more efficient and nimble process operation [16–19]. To enable next-generation or "Smart" operations/manufacturing, novel control methodologies capable of handling dynamic economic optimization of process operations should be designed and investigated. More specifically, there is a need to develop theory, algorithms, and implementation strategies to tightly integrate the layers of Fig. 1.1. The benefits of such work may usher in a new era of dynamic (off steady-state and demand and market-driven) process operations.

In an attempt to integrate economic process optimization and process control as well as realize the possible process performance improvement achieved by consistently dynamic, transient, or time-varying operation, i.e., not forcing the process to operate at a pre-specified steady-state, economic MPC (EMPC) has been proposed which incorporates a general cost function or performance index in its formulation. The cost function may be a direct or indirect reflection of the process economics. However, a by-product of this modification is that EMPC may operate a system in a possibly time-varying fashion to optimize the process economics and may not operate the system at a specified steady-state or target. The notion of time-varying operation will be carefully analyzed throughout this monograph. The rigorous design of EMPC systems that operate large-scale processes in a dynamically optimal fashion while maintaining safe and stable operation of the closed-loop process system is challenging as traditional notions of stability, e.g., asymptotic stability of a steady-state, may not apply to the closed-loop system/process under EMPC. While the concept of using general cost function in MPC has been suggested numerous times in the literature, e.g., [20–23], closed-loop stability and performance under EMPC has only recently been considered and rigorously proved for various EMPC formulations [24–27].

1.2 Tracking Versus Economic Model Predictive Control: A High-Level Overview

A high-level overview of the key differences between tracking and economic MPC is provided. A mathematical discussion of tracking and economic MPC, which requires a formal definition of notation and preliminary results, is delayed until the subsequent chapters. Also, the term tracking MPC is used throughout this monograph to refer to both regulating MPC or MPC formulated to force the process to operate at a given steady-state and tracking MPC or MPC formulated to force the process track a given reference trajectory. Model predictive control, whether tracking or economic, is a feedback control methodology where the control actions that are applied to the closed-loop process/system are computed by repeatedly solving a nonlinear constrained optimization problem on-line. The main components of MPC are:

1. A mathematical model of the process/system to predict the future evolution of the process/system over a time interval called the prediction horizon.
2. A performance index or cost functional that maps the process/system (state and input) trajectories over the prediction horizon to a real number that is a measure of the tracking or economic performance. The cost functional is the objective function of the optimization problem.

3. Constraints on the process/system including restrictions on the control inputs, system states and other considerations, e.g., stability and performance constraints.
4. A receding horizon implementation (described further below).

To make the optimization problem of MPC a finite-dimensional one, the prediction horizon of MPC is typically selected to be finite and the input trajectory over the prediction horizon, which is the decision of the optimization problem, is parameterized by a finite number of variables.

The receding horizon implementation is the strategy that involves repeatedly solving the optimization problem on-line to compute the control actions. Specifically, real-time (continuous-time) is partitioned into discrete time steps called sampling times where the time between two consecutive sampling times is called the sampling period. At each sampling time, the MPC optimization problem is initialized with a state measurement or estimate. The MPC optimization problem is solved to compute the optimal input trajectory over the prediction horizon. The control action(s) computed over the first sampling period of the prediction horizon is/are applied to the closed-loop process/system. At the next sampling time, the MPC problem is resolved after receiving an updated state measurement/estimate. The algorithm is repeated over the length of operation. The receding horizon implementation is important because it introduces feedback to compensate for disturbances, modeling errors, and other forms of uncertainty. Moreover, the receding horizon implementation allows for a better approximation of the solution of the corresponding infinite-horizon optimal control problem, i.e., the MPC problem in the limit as the prediction horizon tends to infinity. The infinite-horizon solution, assuming the solution exists, arguably gives the best solution as chemical processes are typically operated over long periods of time without a natural termination or shutdown time.

Tracking MPC optimization problem takes the following general form:

$$\begin{aligned} &\text{Optimize:} && \text{Tracking cost functional}\\ &\text{Subject to:} && \text{Dynamic model initialized with state measurement/estimate}\\ &&& \text{State/input constraints}\\ &&& \text{Stability constraints} \end{aligned} \tag{1.1}$$

while economic MPC problem takes the following general form:

$$\begin{aligned} &\text{Optimize:} && \text{Economic cost functional}\\ &\text{Subject to:} && \text{Dynamic model initialized with state measurement/estimate}\\ &&& \text{State/input constraints}\\ &&& \text{Economic-oriented constraints}\\ &&& \text{Stability constraints} \end{aligned} \tag{1.2}$$

The main difference between tracking MPC of Eq. 1.1 and economic MPC of Eq. 1.2 is that the tracking MPC problem is formulated with a tracking cost functional, while the economic MPC problem is formulated with an economic cost functional. The tracking cost functional usually uses a quadratic stage cost that penalizes the deviation of state and inputs from their corresponding steady-state, target, or reference values. However, the EMPC cost functional may potentially use any general stage cost that reflects the process/system economics. Since the idea of EMPC is to compute control actions that directly account for the economic performance, economic-oriented constraints may also be added. For example, the economic-oriented constraints may limit the average amount of raw material that may be fed to the process/system or may ensure that the total production of the desired product over a specified length of operation meets demand.

1.3 Chemical Processes and Time-Varying Operation

In this section, a few chemical process examples that will be used to study the closed-loop properties of EMPC are presented to motivate the need for unsteady-state process operation to improve economic performance. As discussed in the introduction, steady-state operation is typically adopted in chemical process industries. In this operating paradigm, the control system is used to force a chemical process to a pre-specified steady-state and maintain operation at this steady-state thereafter until the desired operating steady-state is changed. However, steady-state operation may not necessarily be the best operation strategy with respect to the process economics. In fact, the chemical process control literature is rich with chemical process examples that demonstrate performance improvement with respect to specific cost metrics with dynamic process operation. In particular, many studies have analyzed the economic benefit of periodically operated reactors, e.g., [28–47], and the numerous references therein. To help identify systems that achieve a performance benefit from periodic operation, several techniques have been proposed including frequency response techniques and the application of the maximum principle [28, 36, 48–51]. Periodic control strategies have also been developed for several applications, for instance, [35, 39, 42–44].

While the periodic operating strategies listed above do demonstrate economic performance improvement, in the case of forced periodic operation, i.e., periodic operation induced by periodic switching of manipulated inputs, the periodic operating policies described in many previous works have been identified through a low-order control parameterization, e.g., a bang-bang input profile and in an open-loop fashion. Owing to recent advances in dynamic optimization (numerical solution strategies or direct methods), it is possible that these chemical process examples previously considered in the context of periodic operation may achieve further economic performance improvement under EMPC. Moreover, EMPC may systematically determine, in real-time, the optimal operating strategy based on the current economic factors while meeting operating constraints. When accounting for time-varying economic factors, e.g., real-time energy pricing, and time-varying disturbance, it is certainly possible that more complex operating strategies beyond steady-state and periodic operation are economically optimal. Developing EMPC schemes that dictate such complex operating strategies, which are generally referred to as time-varying operating strategies, has motivated much of the work contained in this book. Two chemical process examples that benefit from time-varying operation are provided below.

1.3.1 Catalytic Oxidation of Ethylene

Consider a benchmark chemical reactor example depicted in Fig. 1.2 that has previously studied in the context of forced periodic operation [38, 39]. Within the reactor, ethylene oxide (C_2H_4O) is produced from the catalytic oxidation of ethylene with air. Ethylene oxide is an important raw material within the chemical industry because it is used for the synthesis of ethylene glycol which is subsequently used to produce many materials. The reactor is modeled as a non-isothermal continuous stirred-tank reactor (CSTR) with a coolant jacket to remove heat from the reactor. Two combustion reactions occur that consume both the reactant and the product, respectively. The reactions are given by

$$
\begin{aligned}
C_2H_4 + \frac{1}{2}O_2 &\xrightarrow{r_1} C_2H_4O \\
C_2H_4 + 3O_2 &\xrightarrow{r_2} 2CO_2 + 2H_2O \\
C_2H_4O + \frac{5}{2}O_2 &\xrightarrow{r_3} 2CO_2 + 2H_2O
\end{aligned}
$$

where r_i, $i = 1, 2, 3$ is the reaction rate of the ith reaction, and the reaction rate expressions are

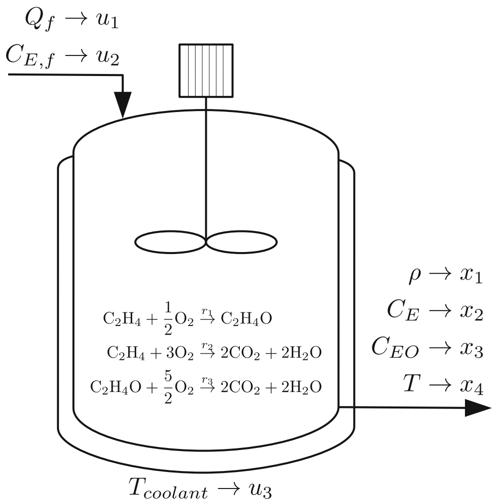

Fig. 1.2 Diagram of the catalytic reactor that produces ethylene oxide from ethylene

$$r_1 = k_1 \exp\left(\frac{-E_1}{RT}\right) P_E^{0.5} \tag{1.3}$$

$$r_2 = k_2 \exp\left(\frac{-E_2}{RT}\right) P_E^{0.25} \tag{1.4}$$

$$r_3 = k_3 \exp\left(\frac{-E_3}{RT}\right) P_{EO}^{0.5} \tag{1.5}$$

where k_i and E_i, $i = 1, 2, 3$ are the reaction rate constant and activation energy for the ith reaction, respectively, T is the temperature, R is the gas constant, and P_j is the partial pressure of the jth component in the reactor ($j = E, EO$ denotes ethylene and ethylene oxide, respectively). The reaction rate expressions are from [52] where catalytic oxidation of ethylene using an unmodified, commercial catalyst was studied over the temperature range 523–573 K. To model the gaseous mixture within the reactor, ideal gas is assumed and the concentration of the jth component within the reactor, denoted by C_j, is

$$C_j = \frac{P_j}{RT}. \tag{1.6}$$

A model describing the dynamic behavior of the reactor is derived through first principles under standard modeling assumptions, e.g., ideal gas and constant heat capacity. The dimensionless states are

$$x_1 = \rho/\rho_{\text{ref}}, \quad x_2 = C_E/C_{\text{ref}}, \quad x_3 = C_{EO}/C_{\text{ref}}, \quad x_4 = T/T_{\text{ref}}$$

where ρ/ρ_{ref} is the dimensionless vapor density in the reactor, C_E/C_{ref} is the dimensionless ethylene concentration in the reactor, C_{EO}/C_{ref} is the dimensionless ethylene oxide concentration in the reactor, and T/T_{ref} is the dimensionless reactor temperature. The manipulated inputs are

$$u_1 = Q_f/Q_{\text{ref}}, \quad u_2 = C_{E,f}/C_{\text{ref}}, \quad u_3 = T_c/T_{\text{ref}}$$

where Q_f/Q_{ref} is the dimensionless volumetric flow rate of the feed, $C_{E,f}/C_{\text{ref}}$ is the dimensionless ethylene concentration of the feed, and T_c/T_{ref} is the dimensionless coolant temperature. The model of the reactor is given by the following set of nonlinear ordinary differential equations:

$$\frac{dx_1}{dt} = u_1(1 - x_1 x_4) \tag{1.7}$$

$$\frac{dx_2}{dt} = u_1(u_2 - x_2 x_4) - A_1 \bar{r}_1(x_2, x_4) - A_2 \bar{r}_2(x_2, x_4) \tag{1.8}$$

$$\frac{dx_3}{dt} = -u_1 x_3 x_4 + A_1 \bar{r}_1(x_2, x_4) - A_3 \bar{r}_3(x_3, x_4) \tag{1.9}$$

$$\frac{dx_4}{dt} = \frac{u_1}{x_1}(1 - x_4) + \frac{B_1}{x_1}\bar{r}_1(x_2, x_4) + \frac{B_2}{x_1}\bar{r}_2(x_2, x_4) + \frac{B_3}{x_1}\bar{r}_3(x_3, x_4) - \frac{B_4}{x_1}(x_4 - u_3) \tag{1.10}$$

where

$$\bar{r}_1(x_2, x_4) = \exp(\gamma_1/x_4)(x_2 x_4)^{1/2} \tag{1.11}$$

$$\bar{r}_2(x_2, x_4) = \exp(\gamma_2/x_4)(x_2 x_4)^{1/4} \tag{1.12}$$

$$\bar{r}_3(x_3, x_4) = \exp(\gamma_3/x_4)(x_3 x_4)^{1/2} \tag{1.13}$$

and the parameters are given in Table 1.1 from [38, 39]. The admissible input values is considered to be bounded in the following sets:

$$u_1 \in [0.0704, 0.7042],$$
$$u_2 \in [0.2465, 2.4648],$$
$$u_3 \in [0.6, 1.1].$$

Following [38], the profitability of the reactor is assumed to scale with the yield of ethylene oxide. Therefore, to optimize the profitability or economics of the reactor, one seeks to maximize the time-averaged yield of ethylene oxide. The time-averaged yield of ethylene oxide over an operating time t_f is given by

Table 1.1 Dimensionless process model parameters of the ethylene oxidation reactor model

Parameter	Value	Parameter	Value
A_1	92.80	B_3	2170.57
A_2	12.66	B_4	7.02
A_3	2412.71	γ_1	–8.13
B_1	7.32	γ_2	–7.12
B_2	10.39	γ_3	–11.07

The parameters are from [38]

$$Y = \frac{\dfrac{1}{t_f}\displaystyle\int_0^{t_f} x_3(\tau)x_4(\tau)u_1(\tau)\,d\tau}{\dfrac{1}{t_f}\displaystyle\int_0^{t_f} u_1(\tau)u_2(\tau)\,d\tau}. \tag{1.14}$$

Since two combustion reactions occur in the reactor that consume both the desired product and the reactant, the yield is a measure of the amount of ethylene oxide leaving the reactor relative to the amount of ethylene fed into the reactor and thus, a good measure for the economic performance of the reactor.

For practical reasons, one may want to optimize the yield while also ensuring that the time-averaged amount of ethylene that is fed to the reactor be fixed, i.e., determine the method to distribute a constant time-averaged amount of ethylene to the reactor that maximizes the yield. Limiting the time-averaged amount of ethylene that may be fed to the reactor is described by the following constraint:

$$\frac{1}{t_f}\int_0^{t_f} u_1(\tau)u_2(\tau)\,d\tau = \dot{M}_E \tag{1.15}$$

where $\dot{M}_E$ is a given time-averaged dimensionless molar flow rate of ethylene that may be fed to the reactor. If $u_{1,\min}u_{2,\min} < \dot{M}_E < u_{1,\max}u_{2,\max}$, the constraint of Eq. 1.15 prevents one from simply considering feeding in the minimum or maximum flow rate of ethylene to the reactor for all time. Within the context of EMPC, the constraint of Eq. 1.15 gives rise to a class of economically motivated constraints which take the form of integral or average constraints. In stark contrast to traditional or conventional control methodologies, e.g., proportional-integral-derivative control or tracking MPC, economically motivated constraints may be directly incorporated into EMPC. As previously mentioned this example has been previously studied within the context of periodic operation, e.g., [38], and closed-loop operation of this reactor under EMPC is considered in later chapters.

1.3.2 Continuously-Stirred Tank Reactor with Second-Order Reaction

A well-known chemical engineering example that demonstrates performance improvement through time-varying operation is a continuously stirred tank reactor (CSTR) where a second-order reaction occurs. Specifically, consider a non-isothermal CSTR where an elementary second-order reaction takes place that converts the reactant A to the desired product B like that depicted in Fig. 1.3. The reactant is fed to the reactor through a feedstock stream with concentration C_{A0}, volumetric flow rate F, and temperature T_0. The CSTR contents are assumed to be spatially uniform, i.e., the contents are well-mixed. Also, the CSTR is assumed to have a static liquid hold-up. A jacket provides/removes heat to/from the reactor at a

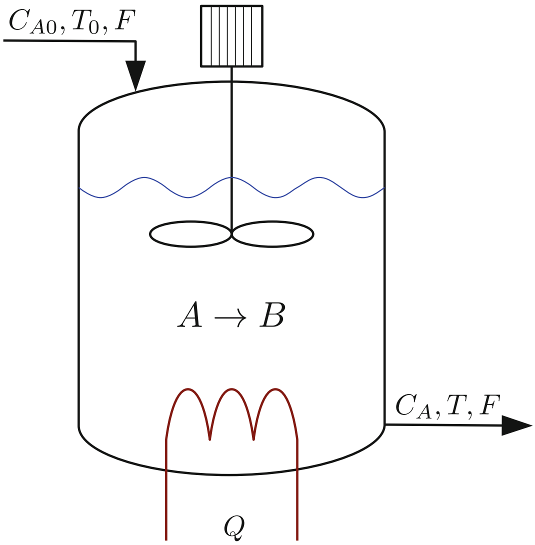

Fig. 1.3 Diagram of a CSTR where a second-order reaction occurs that produces a desired product B from a reactant A

heat rate Q. Applying first principles and standard modeling assumptions, e.g., constant fluid density and heat capacity, which are denoted by ρ_R and C_p, respectively and Arrhenius rate dependence of the reaction rate on temperature, the following system of ordinary differential equations (ODEs) may be obtained that describes the evolution of the CSTR reactant concentration and temperature:

$$\frac{dC_A}{d\bar{t}} = \frac{F}{V_R}(C_{A0} - C_A(\bar{t})) - k_0 e^{-E/RT(\bar{t})}(C_A(\bar{t}))^2 \tag{1.16a}$$

$$\frac{dT}{d\bar{t}} = \frac{F}{V_R}(T_0 - T(\bar{t})) - \frac{(-\Delta H)k_0}{\rho_R C_p} e^{-E/RT(\bar{t})}(C_A(\bar{t}))^2 + \frac{Q}{\rho_R C_p V_R} \tag{1.16b}$$

where $\bar{t}$ is the time, C_A denotes the concentration of A in the reactor, T denotes the temperature of the reactor contents, V_R is the volume of the liquid hold-up in the reactor, k_0 is the rate constant, E is the reaction activation energy, ΔH is the enthalpy of reaction, and R is gas constant.

The ODEs of Eq. 1.16 may be written in dimensionless form by defining $t = \bar{t}F/V_R$, $x_1 = C_A/C_{ref}$, $x_2 = RT/E$, $u = C_{A0}/C_{ref}$, $A_1 = C_{ref}V_R k_0/F$, $A_2 = \Delta H R C_{ref} A_1/(E C_p \rho)$, $x_{20} = RT_0/E + RQ/(C_p \rho E F)$ where C_{ref} is a reference concentration. The resulting dynamic equations in dimensionless form is:

Table 1.2 Process parameters of the CSTR

$k_0 C_{ref}^2$	8.46×10^6	A_1	1.69×10^6
x_{20}	0.050	A_2	1.41×10^4

$$\frac{dx_1}{dt} = -x_1 - A_1 e^{-1/x_2} x_1^2 + u \tag{1.17a}$$

$$\frac{dx_2}{dt} = -x_2 + A_2 e^{-1/x_2} x_1^2 + x_{20} \tag{1.17b}$$

where x_1 is the dimensionless reactant concentration, x_2 is the dimensionless temperature, and A_1, A_2 and x_{20} are constant parameters. The values of the parameters are given in Table 1.2. The input, which is the dimensionless reactant concentration in the reactor inlet, is bounded: $u \in [u_{\min}, u_{max}] = [0.5, 7.5]$. For this example, the production rate of the desired product is assumed to reflect the operating profit of the reactor, which is given by the following function:

$$l_e(x, u) = k_0 C_{ref}^2 e^{-1/x_2} x_1^2. \tag{1.18}$$

Determining the optimal input profile that maximizes the production rate subject to the constraint on the admissible input values is trivial: feed in the maximum amount of material for all time, i.e., set u to u_{max} for all time. A more interesting problem that may lead to a non-trivial solution is to determine the optimal input profile that maximizes the production rate subject to a constraint on the time-averaged amount of material that may fed to the reactor. In the latter problem, a more economical viewpoint is adopted and the problem seeks to determine the optimal method to distribute the material to the reactor. Therefore, the CSTR is assumed to be subject to an input average constraint (dynamic constraint) given by:

$$\frac{1}{t_f} \int_0^{t_f} u(t)\, dt = u_{avg} \tag{1.19}$$

where t_f is the length of operation. For this process (Eq. 1.17), performance metric (Eq. 1.18), and average constraint (Eq. 1.19), forced periodic operation induced by bang-bang type actuation has been shown to improve the average production owing to the second-order dependence of the reaction rate on reactant concentration, e.g., [29–32].

An analysis may be completed to rigorously show that the economic performance, i.e., the average production rate of the product, may be improved by using a time-varying operating strategy (in particular, periodic operation) compared to operating the reactor at steady-state. To show this rigorously, we require some more technical concepts, e.g., the Hamiltonian function, adjoint variables, Pontryagin's maximum principal [53]. Nevertheless, these concepts are not needed later in the book. An auxiliary state is defined for the average constraint:

$$x_3(t) := \frac{1}{t_f} \int_0^t \left(u(t) - u_{avg}\right)\, dt \tag{1.20}$$

which has dynamics:

$$\frac{dx_3(t)}{dt} = \frac{1}{t_f}(u(t) - u_{avg}). \tag{1.21}$$

The non-isothermal CSTR with the stage cost (Eq. 1.18) is a member of a special class of nonlinear systems:

$$\dot{x} = \bar{f}(x) + Bu \tag{1.22}$$

where $\dot{x}$ denotes the time derivative of x, $B \in \mathbb{R}^{n\times m}$ is a constant matrix and $\bar{f} : \mathbb{R}^n \rightarrow \mathbb{R}^n$ is a differentiable vector function. Additionally, the stage cost only depends on the states:

$$l_e(x, u) = \bar{l}_e(x) \tag{1.23}$$

where $\bar{l}_e : \mathbb{R}^n \rightarrow \mathbb{R}$ is a differentiable function. The Hamiltonian function of the system of Eq. 1.22 and cost of Eq. 1.23 is

$$H(x, u, \lambda) = \bar{l}_e(x) + \lambda^T \bar{f}(x) + \lambda^T Bu \tag{1.24}$$

where λ is the adjoint variable vector that satisfies

$$\dot{\lambda}(t) = -H_x(x(t), u(t), \lambda(t)) \tag{1.25}$$

where H_x denotes the partial derivative of H with respect to x. From Pontryagin's maximum principle [53], a necessary condition can be derived for the optimal control, i.e., the control that maximizes the Hamiltonian:

$$u_i^*(t) = \begin{cases} u_{i,\max}, & \text{if } b_i^T \lambda(t) > 0 \\ u_{i,\min}, & \text{if } b_i^T \lambda(t) < 0 \end{cases} \tag{1.26}$$

where b_i is the i-th column of B. For this class of systems and stage costs, if some time-varying operating policy is the optimal operating strategy, then the operating policy is a bang-bang input policy of Eq. 1.26.

Although the analysis above significantly reduces the space of possible optimal input trajectories, it still yields an infinite space of input trajectories. Thus, consider the following periodic bang-bang input trajectory over one period:

$$u(t) = \begin{cases} u_{\max} & \text{if } t < \tau/2 \\ u_{\min} & \text{else} \end{cases} \tag{1.27}$$

where τ is the period and $t \in [0, \tau)$. The input trajectory of Eq. 1.27 satisfies the average constraint of Eq. 1.19 over each period (in this regard, the length of operation,

t_f, is assumed to be a multiple of τ). For the system of Eq. 1.17 with the input trajectory of Eq. 1.27, there exists a periodic state trajectory for some $\tau > 0$, i.e., it has the property $x(t) = x(t + \tau)$ for all t.

In this example, u_{avg} is taken to be 4.0. The CSTR has an optimal steady-state $x_s^T = [1.182 \;\; 0.073]$ which corresponds to the steady-state input that satisfies the average input constraint ($u_s = u_{avg}$) with a production rate of 14.03. Indeed, the periodic solution of the system of Eq. 1.17 with the input of Eq. 1.27 achieves better economic performance compared to the economic performance at steady-state for some τ. Moreover, the economic performance depends on the period which is shown in Fig. 1.4. Over the range of periods considered (0.5 to 2.4), the period $\tau = 1.20$ yields the best performance (Fig. 1.4). The periodic solution with the input period of $\tau = 1.20$ has an average cost of $\bar{J}_e = 15.20$ which is 8.30 percent better than the performance at the optimal steady-state. Periods greater than 1.96 achieve worse performance compared to that at steady-state. The state, input, and $B^T\lambda = b_1^T\lambda = \lambda_1 + \lambda_3/\tau$ trajectories are given in Fig. 1.5 over one period. From Fig. 1.5, the input trajectory satisfies the necessary condition of Eq. 1.26. From these results, time-varying operation is better than steady-state operation from an economical point of view for this example. If the average constraint of Eq. 1.19 was not imposed, the optimal operating strategy would be steady-state operation at the steady-state corresponding to the input $u_{\max}$. The average constraint plays a crucial role for this particular example.

As pointed out, the above analysis only considers economic performance. If the periodic solution depicted in Fig. 1.5 is indeed optimal or some other bang-bang policy is the best operating strategy, feedback control is needed to force the system state from an initial state to the optimal time-varying solution. Moreover, the control problem becomes more complex when one considers disturbances, plant-

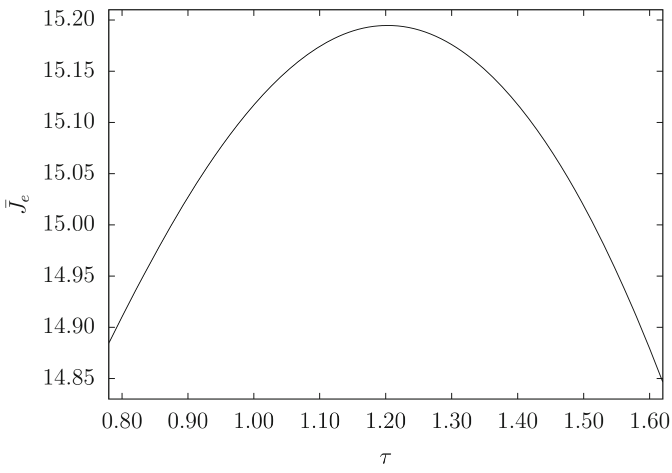

Fig. 1.4 Average economic performance $\bar{J}_e$ as a function of the period length τ

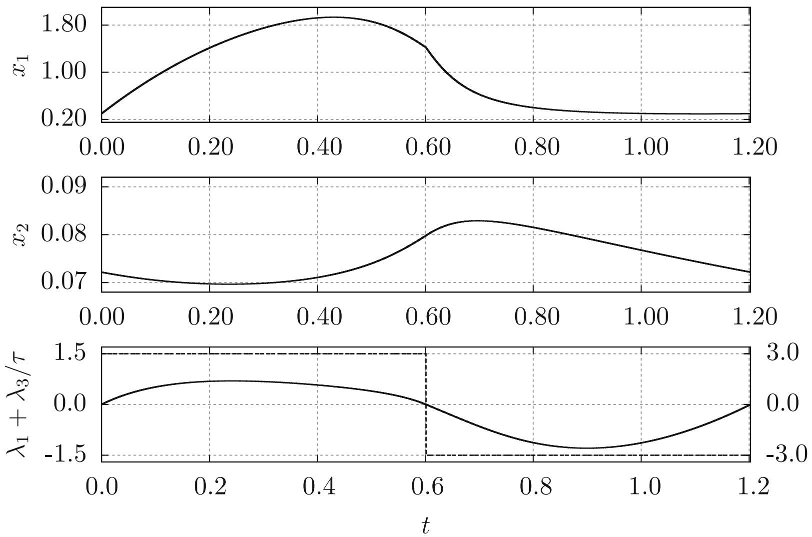

Fig. 1.5 State, input, and $\lambda_1 + \lambda_3/\tau$ trajectories of the CSTR under the bang-bang input policy with period $\tau = 1.20$

model mismatch and other forms of uncertainty, implementability of the computed input trajectory, i.e., bang-bang control may not be implementable in practice, and time-varying economic objectives and constraints. The example further motivates the inquiry and theoretical developments in the context of EMPC systems that dictate time-varying operating policies.

1.4 Objectives and Organization of the Book

This book considers theoretical analysis of closed-loop stability and performance under EMPC, issues related to computational efficiency of EMPC, and chemical process applications controlled by EMPC. Specifically, the objectives of this book are summarized as follows:

1. To develop economic model predictive control methods that address infinite-time and finite-time closed-loop economic performance and time-varying economic considerations.
2. To develop two-layer dynamic economic process optimization and feedback control frameworks that incorporate EMPC with other control strategies allowing for computational efficiency.
3. To develop rigorous output feedback-based EMPC schemes with guaranteed closed-loop stability properties.
4. To address real-time computation of EMPC.

The book is organized as follows. In Chap. 2, a formal definition of the notation is provided. Some definitions and preliminary results on stability and stabilization of nonlinear systems and on tracking MPC are given. The chapter closes with a brief review of nonlinear constrained optimization and solution strategies for dynamic optimization.

In Chap. 3, a brief overview of EMPC methods is provided. In particular, the role of constraints imposed in the optimization problem of EMPC for feasibility, closed-loop stability, and closed-loop performance is explained. Three main types of constraints are considered including terminal equality constraints, terminal region constraints, and constraints designed via Lyapunov-based techniques. EMPC is applied to a benchmark chemical process example to illustrate the effectiveness of time-varying operation to improve closed-loop economic performance compared to steady-state operation and to an open-loop periodic operating policy.

In Chap. 4, a complete discussion of Lyapunov-based EMPC (LEMPC), which was first presented in [27], is given that includes closed-loop stability and robustness properties. LEMPC designs that address closed-loop performance and time-varying economic stage cost function are also addressed in this chapter. The methods are applied to two chemical process examples.

In Chap. 5, output feedback-based EMPC schemes are presented. To provide EMPC with an estimate of the system state from a measurement of the output, a high-gain observer and moving horizon estimation (MHE) are both considered for state estimation. Conditions under which closed-loop stability under the two resulting state estimation-based EMPC schemes are derived. The state estimation-based EMPC schemes are applied to a chemical process example.

In Chap. 6, several two-layer approaches to dynamic economic optimization and control are developed and discussed. The upper layer, utilizing an EMPC, is used to compute economically optimal policies and potentially, also, control actions that are applied to the closed-loop system. The economically optimal policies are sent down to a lower layer MPC scheme which may be a tracking MPC or an EMPC. The lower layer MPC scheme forces the closed-loop state to closely follow the economically optimal policy computed in the upper layer EMPC. The methodologies are applied to several chemical process examples to demonstrate their effectiveness.

In Chap. 7, issues relating to computational efficiency and real-time implementation of EMPC are addressed. First, a composite control structure featuring EMPC is developed for nonlinear two-time-scale systems. The resulting control strategy addresses computational efficiency because it is a distributed control strategy and it has certain numerical advantages explained further in the chapter. Next, an alternative to solving for the control actions for all available inputs in a single optimization problem is discussed. Specifically, several (smaller) optimization problems may formulated and solved to compute the control actions that are applied to the closed-loop system. Owing to the fact that the optimization problems are solved amongst several distributed processors, the resulting strategy is a distributed EMPC (DEMPC) implementation. In this chapter, an application study of DEMPC is presented. Two DEMPC approaches are considered and evaluated with respect to a centralized EMPC implementation. Finally, to address guaranteed closed-loop stability in the presence of computational delay, an implementation strategy is developed which features a triggered evaluation of the LEMPC optimization problem to compute an input trajectory over a finite-time prediction horizon in advance. Closed-loop stability under the real-time LEMPC strategy is analyzed and specific stability conditions are derived.

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