DESIGN AND ANALYSIS OF DYNAMIC REAL-TIME OPTIMIZATION SYSTEMS

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by

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ABSTRACT

Process economic improvement subject to safety, operational and environmental constraints is an ultimate goal of using on-line process optimization and control techniques. The dynamic nature of present-day market conditions motivates the consideration of process dynamics within the economic optimization calculation. Two key paradigms for implementing real-time dynamic economic optimization are a dynamic real-time optimization (DRTO) and regulatory MPC two-layer architecture, and a single-level economic model predictive control (EMPC) configuration. In the two-layer architecture the economically optimal set-point trajectories computed in an upper DRTO layer are provided to the MPC layer, while in the single-layer EMPC configuration the economics are incorporated within the MPC objective function. There are limited studies on a systematic performance comparison between these two approaches. Furthermore, these studies do not simultaneously consider the economic, disturbance rejection and computational performance criteria. Thus, it may not be clear under what conditions one particular method is preferable over the other. These reasons motivate a more comprehensive comparison between the two paradigms, with both open- and closed-loop predictions considered in the DRTO calculations. In order to conduct this comparison we utilize two process case studies for the economic analysis and performance comparison of on-line optimization systems. The first case study is a process involving two stirred-tank reactors in-series with an intermediate mixing point, and the second case study is a linear multi-input single-output (MISO) system. These processes are represented using a first principles model in the form of differential-algebraic equations (DAEs) system for the first case study and a simplified linear model of a polymerization reactor for the second case study problem. Both of the case study processes include constraints associated with input variables, safety considerations, and output quality. In these case study problems, the objective of optimal process operation is net profit improvement.

The following performance evaluation criteria are considered in this study: (I) optimal value of the economic objective function, (II) average run time (ART) over a same operating time interval, (III) cumulative output constraint violation (COCV) for each constraint. The update time of the single-layer approach is selected to be equal to that of the control layer in

the two-layer formulations, while the update time of the economic layer in the two-layer formulation is bigger than that of the single-layer approach. The nonlinear programing (NLP) problems which result in the single-layer and two-layer formulations and the quadratic programing problem which corresponds to the MPC formulation are solved using the fmincon and quadprog optimization solvers in MATLAB. Performance assessment of the single-layer and two-layer formulations is evaluated in the presence of a variety of unknown disturbance scenarios for the first case study problem. The effect of a dynamic transition in the product quality is considered in the performance comparison of the single-layer and two-layer methods in the second case-study problem.

The first case study problem results show that for all unknown disturbance scenarios, the economic performance of the single-layer approach is slightly higher than that of the two-layer formulations. However, the average computation time for the DRTO-MPC two-layer formulations are at least one order of magnitude lower than that of the EMPC formulation. Also, comparison results of the COCV for the EMPC formulation for different sizes of update time intervals could justify the necessity of the MPC control layer to reduce the COCV for the economic optimization problems with update times larger than that of the MPC control layer. A similar computational advantage of the OL- and CL-DRTO-MPC over the EMPC is observed for the second case study problem. In particular it is shown that increasing the economic horizon length in the EMPC formulation to a sufficiently large value may result a higher economic improvement. However, the increase in economic optimization horizon would increase the resulting NLP problem size. The computational burden could limit the use of the EMPC formulation with larger economic optimization horizons in real-time applications. The ART of the dual-layer methods is at least two orders of magnitude lower than that of the EMPC methods with an appropriate horizon length. The CL-DRTO-MPC economic performance is slightly less than that of the EMPC formulation with the same economic optimization horizon.

In conclusion, the performance comparison on the basis of multiple criteria in this study demonstrates that the economic performance criterion is not necessarily the only important metric, and the operational constraint limitations and the optimization problem solution time could have an important impact on the selection of the most suitable real-time optimization approach.

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I wish to express my gratitude to my supervisor, Dr. Christopher Swartz, for his support, advice and guidance throughout the course of this research. This thesis would certainly not be possible without his patience, vision, and direction.

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This thesis is dedicated to my wife, Leila and my parents for their support all these years, particularly during the difficult periods of my life.

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Chapter 1

Introduction

Real-time operations optimization (RTO) is an on-line technique to improve process operation characteristics such as process profit, yield, reaction selectivity and/ or conversion subject to the environmental, safety and quality considerations. This method uses a rigorous steady state process model and measurement feedback to maximize an economic objective function of the processes. The RTO optimizing input variables could be determined by the solution of an NLP problem (Marlin *et al.* [1997]). In many process operations dynamic changes could provide additional degrees of freedom for the improvement of the process operation (Tosukhowong *et al.* [2004]). The dynamic nature of present-day market conditions; dynamic transitions in product grade and operating conditions including long-lasting dynamics of the processes; and persistent disturbance changes that have a major impact on the process economics, motivates the consideration of the process dynamics within the economic optimization calculation. The necessity of including process dynamics in RTO methods has led to the development of dynamic real-time optimization (DRTO) formulations (Klatt *et al.* [2000], Zanin *et al.* [2002], Engell [2007], Kadam and Marquardt [2007], and Ochoa *et al.* [2010]). Considering the automation decision hierarchy, economically optimal set-point trajectories computed in an upper DRTO layer are provided to an advanced control layer which uses a multi-input multi-output (MIMO) control strategy. Process regulation and safety goals could be met at this control level (Marlin *et al.* [1997]).

A linear MPC controller formulation is commonly considered for the advanced control layer (Tosukhowong *et al.* [2004]). This control method uses a quadratic objective function to minimize the deviation of the inputs and outputs of the process from their set-points using a linearized model prediction of the process (Rawlings and Mayne [2009]). There is another alternative for the real-time operation of the chemical processes in which economics are incorporated within an EMPC objective function (Amrit *et al.* [2013]). The resulting economically optimal control architecture involves unifying the target setting function and the regulator function in a single-level (Bartusiak [2007]).

1.1 Problem Motivation and Goals

Recently, the single-level approach attracted considerable attention within the control community, (for example see Ellis *et al.* [2014a] and the references therein). The EMPC approach could be considered as a promising replacement for the DRTO-MPC formulation because there is no time-scale separation problem and model inconsistency issues which could exist between in the RTO and control layer in the two-layer counterpart of the EMPC (Rawlings and Amrit [2009]). However, the single-layer structure needs to be implemented with the same frequency of control layer in the hierarchical structure to account for the control task as well as the economic improvement task. Hence, the single-layer economic optimization updating rate is naturally faster than that of the RTO layer in the two-layer structure. In addition, a large economic optimization horizon might be needed to achieve an economic performance improvements (Ellis and Christofides [2014b]). The large economic optimization horizon could significantly increase the problem size. A large problem size may limit the real-time application of the EMPC formulation due to the undesired effects of computational delay such as diminished economic performance and stability issues (Yang and Biegler [2013]). Thus, it may cause unnecessary and costly computations in cases where only the slow-varying modes of the system and low frequency disturbances have a dominant effect on the process economics. In these cases, the two-layer approach might be useful to reduce computational effort via a slower update of the setpoint in the RTO layer; while the inner control layer is responsible for the regulation of the fast varying modes of the system and disturbances. This expectation could be explored by comparing the single-layer and two-layer method's economic and computational performance to demonstrate the possibility of achieving an equivalent economic operation with a lower computational cost in the two-layer methods.

There are few researchers who have compared the performance of the two current approaches on the basis of the computational, economic and operational criteria. For instance, Ochoa *et al.* [2010] compared a pure economic formulation of the single-layer approach with an open-loop two-layer D-RTO structure for an extractive alcoholic fermentation process. As an other example, Tosukhowong *et al.*, 2004 compared the economic performance of three different two-layer RTO/decentralized MPC formulations for a reactor-storage tank-separator and recycle (RSSR) process system. Systematic performance comparisons between these two strategies are limited to the open-loop DRTO-MPC formulations and do not simultaneously consider economic, disturbance rejection and computational performance criteria. An inclusive and detailed discussion of these comparison studies are included in chapter 2. This fact motivates a systematic performance comparison for the single-layer EMPC and dual-layer DRTO-MPC architectures, with both open- and closed-loop flavours of the prediction considered in the DRTO calculation (Jamaludin and Swartz [2017b]). A review of the open- and closed-loop prediction of the DRTO calculation is included in the literature review part of the thesis in chapter 2 and the general formulation is addressed in chapter 3.

1.2 Research Approach and Scope

Potential process candidates which could benefit from the two-layer D-RTO and economic model predictive control (EMPC) methods have dynamic and operating characteristics such as switching conditions, frequent transitions, slow-varying dynamics, sustained disturbances and high interaction between process units such as large recycle/feed ratio or mass/energy integration loops (Tosukhowong *et al.* [2004]). These process characteristics could provide insight for consideration of appropriate process candidates for our comparison study. Considering these characteristics, one of the reasonable choices for a realistic case study problem is the extractive alcoholic fermentation used by Ochoa *et al.* [2010] for the single-layer and two-layer DRTO comparison. However, the process model and the associated parameters are not explicitly available in their study and the other relevant references. Lack of a clear process model causes a difficulty in the reproduction of the simulation results. The chosen process model candidates are two benchmark models which are used in the literature either to study the performance of the real-time optimization methods or to compare the computational and economic performance of the open- and closed-loop dynamic RTO methods. Also, all of the details for the models are available in the reference papers to reproduce the previous simulation results. The first case study problem is a nonlinear differential-algebraic equation (DAE) system of two stirred-tank reactors (CSTRs) in series with an intermediate feed (Loeblein and Perkins [1998]) and the second case study is a linear multi-input single-output (MISO) system (Jamaludin and Swartz [2017a]). There are constraints on the input variables, safety considerations, and output quality in both of the case study problems. The existence of the output constraints could be considered as a reason to justify the necessity of the control layer use in the implementation of the two-layer structure. The economic optimization objective of the case study problems is the net profit improvement and is denominated in dollar terms.

A fixed and sufficiently long economic optimization horizon is considered for all of the formulations. For the control layer of the two-layer approaches, a standard linear model predictive control (MPC) formulation with a sufficiently long prediction horizon to maintain stability is used. The single-layer approach sample time is selected to be equal to that of the control layer update time in the two-layer methods. In the solution step, a sequential method is used to obtain the dynamic model solution in each iteration step of the resulting nonlinear programming problem (NLP). Open- and closed-loop prediction strategies are considered in the DRTO layer of two-layer DRTO-MPC formulations. The open-loop DRTO (OL-DRTO) layer uses the process model for the process output predictions whereas, the closed-loop DRTO (CL-DRTO) layer uses embedded MPC subproblems in addition to the process model. The focus of this thesis is on the formulation and the implementation of the EMPC and OL- and CL-DRTO-MPC systems for the purpose of performance comparison, hence it does not aim to go through the detailed theory of the optimization solution methods. Therefore, the resulting NLP and QP problems are solved using fmincon and quadprog optimization solvers in MATLAB. For the first case study problem, the performance assessment of the single-layer and two-layer formulations is repeated in the presence of four unknown disturbance scenarios of the fresh feed concentration and the coolant flow rate of the first reactor system. These designated unknown disturbance scenarios are in the form of a variety of short-term and sustained pulse signals. Also, a product grade transition is considered for the second case study problem. Most of integrated plants have very long transient dynamics due to the presence of recycle loops (Tosukhowong [2006]). A large economic optimization horizon might be needed to capture the effect of the long transient dynamics on the economic improvement. As mentioned earlier, a large economic horizon could cause difficulty for the real-time implementation of EMPC formulation. This possible difficulty motivates us to consider recycle effects in the second case study problem. For linear systems these recycle effects could be reflected in a form of change in the process time constant and steady state input-output gains (Luyben [1993]).

The optimal value of the economic objective function, average run time (ART) over the biggest update time intervals among the different formulations and the cumulative output constraint violation (COCV) for each constraint, are considered for the performance evaluation. The third metric is used to quantify constraint violation in the performance comparison in the first case study problem and to justify the necessity of the control layer in the two-layer approaches for the regulation task.

1.3 Main Contributions

As a main contribution, a systematic performance comparison for the single-layer EMPC and dual-layer DRTO-MPC architectures is conducted using two different case study problems. There are some unique aspects of this comparison study that could distinguish it from the existing literature on the performance comparison of the existing EMPC and DRTO approaches. Multiple performance criteria for the DRTO and EMPC schemes are evaluated for the dynamic transition problem and a variety of short-term and sustained unknown process disturbances. Also, both open-loop DRTO (OL-DRTO) and closed-loop DRTO (CL-DRTO) prediction methods are considered in the performance comparison. Another key outcome of this comparison is an order of magnitude reduction in the computational time of the economic optimization using the DRTO approaches for an approximately equivalent economic improvement.

Simultaneous and sequential methods are two main approaches for solving optimization problems that include a dynamic model (see chapter 2 for a detailed review of these methods). In the simultaneous method the dynamic model is discretized together with the manipulated input variables. Whereas, in the sequential dynamic optimization, the dynamic model of the process must be integrated using an ODE solver in each function evaluation of the economic and control problems. The CL-DRTO-MPC formulation is originally developed based on the simultaneous solution approach. However, in this study a sequential optimization framework is chosen to avoid a large optimization problem size in the single-layer and two-layer approaches. Therefore, development and implementation of the CL-DRTO-MPC approach in a sequential optimization framework is the second main contribution of this study.

1.4 Thesis Overview

The contents of this thesis are coordinated in the following chapters:

Chapter 2 – Literature Review In this chapter relevant background on the economic optimization of process plant operation which leads to the thesis research objectives is included. The basic principle of the RTO method and some of its primary charachteristics are discussed in the first section. In the next section, recent developments of the standard formulation for the RTO and EMPC are included. This section is followed by the current status of the economic optimization methods in terms of their advantages and disadvantages in the process industries. Considering the existing issues in the applicability of the single-level EMPC and the two-layer DRTO-MPC formulations, some of the open questions are discussed in the last section. These issues are considered in context of active research directions such as performance comparison and time-scale separation. Also, the significance of each research direction is explained in the last section.

Chapter 3 – Formulation and Comparison methodologies

This chapter describes a selected single-layer EMPC formulation and OL-DRTO formulations. Moreover, it provides a sequential solution framework which is developed for the inclusion of the CL-DRTO formulation in the performance comparison of economic optimization methods. In addition to the problem formulation, this chapter introduces the comparison critera and presents crucial assumptions which are considered in the EMPC and OL- and CL-DRTO design and implementation.

Chapter 4 – First Case Study Problem

This chapter begins with a brief description of the case study problem. The process description is followed by the fundamental DAE process model and the operational constraints. Also, the economic objective function and different sources of the unknown process disturbances are described. Design and tuning parameters are reviewed and the performance results analyzed and discussed for the EMPC, OL-DRTO-MPC and the CL-DRTO architectures, with relevant graphs and tables presented in the last part of this chapter.

Chapter 5 – Second Case Study Problem

This chapter begins with a brief description of the case study problem, the economic objective function and constraints. The solution strategies for the single- and dual-layer methods are reviewed and results of the proposed sequential solution method for the OL- and CL-DRTO formulations are compared with the results of Jamaludin and Swartz [2017a]. Then, the detuning economic performance effects for some of the design parameters are investigated, and suitable design parameters are selected for the performance comparison of the EMPC and dual-layer methods. Finally, the recycle effect on the linear system is considered in a performance comparison of the economic optimization problems and the results are discussed.

Chapter 6 – Conclusions and Recommendations

At the end of this study, the key outcomes of performance comparison results for the case study processes are included. These results are followed by conclusions on conditions under which the two-layer methods could possibly be more preferable to the EMPC formulation from the computational, operational and economic points of view. In this part the necessity of considering multiple performance criteria for the selection of a suitable real-time optimization approach is emphasized. Also, the results of the performance analysis for the suggested sequential formulation of the CL-DRTO approach are mentioned and some remarks on the application of the closed-loop method for a better performance in comparison to the other methods are included.

Chapter 2

Literature Review

2.1 On-line Economic Optimization Approaches

Reducing operational costs in competitive production, complying with environmental constraints, meeting different product specifications, and handling continuous changes in surrounding, utility, operational, feedstock conditions, energy price changes and product demand forecasts are all indispensable for efficient and profitable plant operation. These goals could be accomplished through appropriate online optimization and control algorithms. There are two general categories of methods to achieve optimal operation of process plant systems: (I) hierarchical two-layer real time optimization (RTO) approach and (II) single-layer economic optimization approach. The former takes the form of a cascade structure between the RTO and control layers. In the latter, online optimization is implemented in a single layer and there is no need to control the system to a given setpoint in a separate control layer. A general schematic of these two architectures is depicted in figure 2.1. There are a variety of different two-layer and single-layer approaches in the literature. In this section, these methods are briefly reviewed.

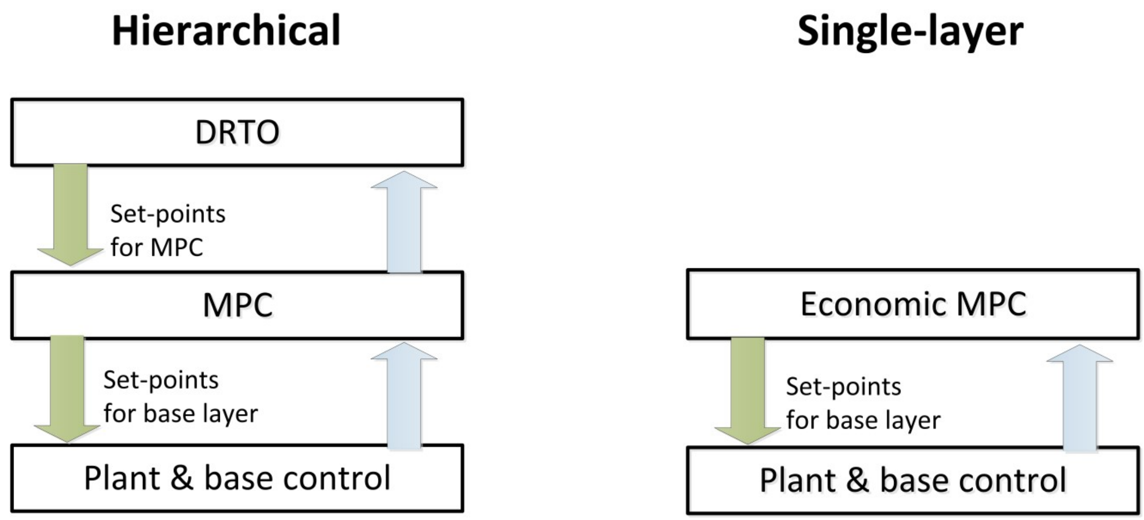

Figure 2.1: Two-layer and single-layer architectures of optimal process operation in the automation decision hierarchy.

2.1.1 Two-layer DRTO Approach

This approach determines economically optimal setpoints in an outer layer using an online feedback optimization strategy in equation 2.1.

$$\begin{aligned}
\underset{U_{ss},X_{ss}}{\text{maximize}} \quad & \Phi_{eco}(X_{ss}, U_{ss}, C(k)) \\
\text{subject to} \quad & 0 = F(X_{ss}, U_{ss}, d; \theta) \\
& G(X_{ss}, U_{ss}) \leq 0
\end{aligned} \tag{2.1}$$

where Φ_{eco} is the economic objective as a function of the stationary input U_{ss} and state variables X_{ss} which are the decision variables in the optimization problem. It is also a function of cost parameters C which could change in each RTO iteration step. The equality constraint F is the rigorous steady state model of the process which is a function of the input and state variables and the unknown disturbance scenarios d and the model parameters θ. The inequality constraint could be a general representation of the input and output constraints, and any other possible operational constraints.

Then in an inner layer of the two-layer approach, an MPC control formulation regulates the system around the optimal setpoints which are the solution of the economic optimization problem in equation 2.1. According to Marlin *et al.* [1997], conventional RTO approaches use a steady state process model to find the optimal operating point. This may lead to a deficiency when the external conditions change more frequently and/or the slow transient changes in the state variables have a significant effect on the process economics. Some researchers proposed the idea of replacing the steady state model with a dynamic process model in the optimization layer to overcome these problems (Klatt *et al.* [2000], Zanin *et al.* [2002], Engell [2007], Kadam and Marquardt [2007], and Ochoa *et al.* [2010]). However, drawbacks associated with the two-layer approach, are model inconsistency between the optimization layer and control layer, and the necessity to deal with time scale separation in the design of the DRTO and predictive control layers (Rawlings and Amrit [2009]). The single-layer economic optimization alternative combines the economic optimization problem and regulatory control problem of the two-layer approaches approach to avoid the model inconsistency and time-scale separation problems. This method uses an idea of the receding horizon optimization similar to the model predictive control (MPC) formulation. A more detailed description of the single-layer method is included in the next section.

2.1.2 Single-layer Approach

In the standard MPC formulation, control actions are calculated by solving an on-line constrained optimization problem at each sample time. This optimization problem minimizes a quadratic objective function for a finite prediction time horizon subject to some constraints on the states and control actions. Using the MPC formulation it is possible to integrate economic optimization and control layers as a unified direct optimizing control layer. This possibility presents MPC as an alternative to the two-layer approach (Rawlings and Amrit [2009]). In the single-layer approach, the quadratic objective function of the MPC formulation is replaced with either a pure economic objective function or a combination of the economic and control objective functions. The economic objective function describes a criterion such as profit, productivity, selectivity, yield, etc (Ellis *et al.* [2014a]). As a result of this change in the objective function, solution of the optimization problem provides input actions for the optimal operation of the plant. Despite the fact that single-layer approach eliminates controller layer, it still has some challenging issues. For instance, in comparison with the economic optimization layer of the two-layer approach, this method requires a higher frequency of solving an economic dynamic optimization problem which could increase the computational effort in comparison to the two-layer method; there is no general stability analysis; and also it has reliability issues (Rawlings and Amrit [2009]). The reliability problem means that there is no back up control system in the case of failure for the single-layer economic control (Ochoa *et al.* [2010]). Moreover, some of the common single-layer formulations use an a-priori known fixed setpoint (Angeli *et al.* [2012] and Heidarinejad *et al.* [2012a]), which may result in suboptimal transitions.

2.2 Active Research Directions

There has been some progress in the improvement of the single- and dual-layer approaches. These advances have focused mostly on the stability analysis of the single-layer approach, solution for the model inconsistency issues in the two-layer approach, reduction of the computational demands and development of faster optimization strategies for the dynamic optimization problem in both methods.

2.2.1 Performance Comparison of the Standard Formulations

As mentioned in the previous section, the single-layer structure needs to be implemented at the same frequency as control layer in the hierarchical structure to account for the control task as well as economic optimization. Hence, the single-layer updating rate is naturally faster than the RTO layer in the two-layer structure. Thus, it may cause unnecessary and costly computations in the cases that only the slow-varying modes of the system and low frequency disturbances have a dominant effect on the process economics. In these cases, the two-layer approach might be useful to reduce the computational effort via a slower update of the setpoint in the RTO layer; while the inner control layer is responsible for fast varying modes of the system and disturbances. This strategy needs to be explored by comparing the single-layer and two-layer methods' economic and computational performance to investigate whether an equivalent economic operation can be achieved with a lower computational cost.

There are few researchers who have compared performance of the two current approaches to illustrate the computational, economic and operational advantages of the single-layer and two-layer approaches for different processes. For instance, Ochoa *et al.* [2010] have compared a pure economic formulation of the single-layer approach with a two-layer D-RTO structure for an extractive alcoholic fermentation process. They maximize productivity of ethanol production in a process system of fermentor, flash separator with a recycle stream. In this process, the system flow rate of the flash separator to fermentor recycle stream and the fermentor input flow rates of starch and enzyme are manipulated variables. Biomass and ethanol concentration of the fermentor are considered as dynamic variables and starch feed concentration is a process disturbance. They concluded that the single-layer approach gives higher productivity for the process. However they did not provide the same conditions for the implementation of the single-layer and two-layer D-RTO approaches. The following remark should be considered for a fair comparison of the two approaches in their case study process:

- They chose an update time of 0.5 hour for both of the single-layer approach and DRTO layer in the two-layer approach and 0.2 hour for the control layer update time, as it is assumed in their study update frequency of the DRTO layer should generally be lower than the update frequency of the control layer in the two-layer DRTO structure. However, the update time of the direct optimizing control should preferably be chosen equal to that of the inner control layer of DRTO method for better consistency. These two criteria are necessary to handle fast-varying modes and disturbances in the system. Therefore in their implementation the necessity of using the control layer in the two layer approach may not be justifiable, resulting in an increase in computational burden without any outcome. Ochoa *et al.* [2010]'s comparison results confirm that controlling biomass concentration to a fixed setpoint using the inner control layer cause economic performance deterioration. A successful justification of the necessity for the controller means that the direct optimizing control should be susceptible to the fast changes in the process modes and disturbances. In this regard the researchers explain that single-layer method has a ”dead period” between update times. They claim that if a disturbance affects the process during this ”dead period”, it may drive the process to a condition of poor performance, and this will not be corrected until the following optimization task is triggered. However they did not consider a scenario in their case study simulation to show that the economic performance in the single layer method decreases in the presence of disturbances.

In addition, Tosukhowong *et al.*, 2004 have compared economic performance of three different two-layer RTO/decentralized MPC formulations for a reactor-storage tank-separator and recycle (RSSR) process system. They intended to justify necessity of DRTO in cases where implementation of steady state RTO (SS-RTO) is not possible and/ or does not provide expected improvement. However in their study, there is no performance analysis of the single-layer real time optimization approach to specify which structure is a suitable option to be implemented for a certain type of process system. Therefore, in the next chapters, we will develop a systematic comparison of a two-layer D-RTO strategy versus a single-layer formulation, in order to infer the conditions under which a certain approach is preferable over the other.

2.2.2 Model Inconsistency Moderation

Model inconsistency arises for some reasons such as using different models for the optimization and control layers, or avoiding closed loop control effects in the optimization layer. Jamaludin and Swartz [2017b] developed a closed-loop two-layer formulation to capture the closed-loop control effect in the optimization layer.

2.2.3 Handling Uncertainty Using a Robust EMPC Formulation

There are two different approaches in dealing with model parameter and economic uncertainty. The first approach is to estimate or predict uncertainties. Huang [2010] tried to estimate the uncertain model parameters and the fictitious process noise for the purpose of performance improvement in some RTO applications. Also, Würth *et al.* [2011] suggested the use of disturbance trend detection in a two-layer DRTO formulation to improve the economic performance. The second approach is application of stochastic optimization methods (e.g. Min-max MPC, multi-stage NMPC). Lucia *et al.* [2013] applied a multi-stage MPC formulation for the control of a semi-batch polymerization reactor under uncertainty. Following this successful application of the multi-stage MPC formulation to handle the process model parameter uncertainty, later they incorporated this robust MPC technique in economic model predictive control (Lucia *et al.* [2014]). In this method an uncertainty horizon tree is considered which should be obtained using process knowledge and/ or statistical methods (see figure 2.2). In this figure d_i^js are j different possibilities for the disturbance in time instance i. Also u_i^j is jth input element in time instance i which results jth predicted state in the next time instance. From figure 2.2 one can infer that adding a longer horizon will result a larger optimization problem. For instance, there are three generations of the child nodes in the following scenario tree and the horizon size is $N = 3$. However, there are some basic methods to limit the scenario options after a certain horizon length.

2.2.4 Integration with the Estimation Techniques

Similar to conventional feedback control systems, in the development of online optimization methods, it is typically assumed that all state variables are available. In fact, it is not always possible to measure all state variables. Therefore, states of the system could be estimated using an appropriate estimation method. One approach is to use high gain observer with guaranteed closed-loop stability. Heidarinejad *et al.* [2012b] used a high-gain observer to extend the use of a Lyapunov based model predictive control (LEMPC) method for the case that the full state measurements are not available. According to Ellis *et al.* [2014a], this

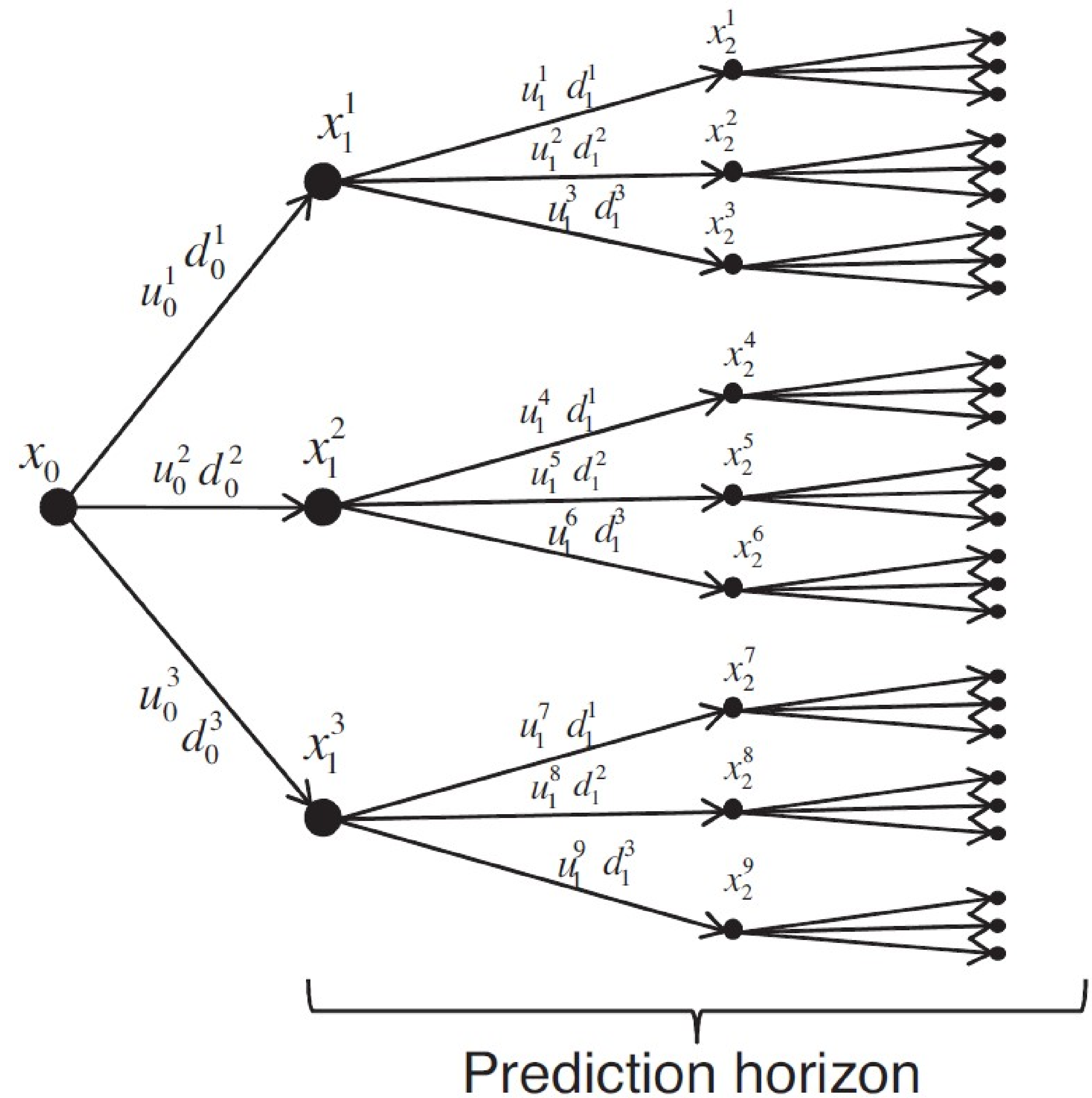

Figure 2.2: Scenario tree representation of the uncertainty evolution (adapted from Lucia *et al.* [2013]).

type of estimator cannot handle constraints and it may also be sensitive to measurement noise. The other option is Extended Kalman Filter (EKF) which is an optimization-based state estimation method, which can account for noise. Rawlings and Mayne [2009] claimed that "EKF is at best an ad-hoc solution to a nonlinear state estimation problem". Thus, it can fail due to inaccurate linearization and cannot handle constraints reliably. To escape the possible pitfalls of EKF, the Unscented Kalman Filter (UKF) has been introduced. This method uses several samples of the nonlinear response, called sigma points, to avoid linearization. In addition, it accounts for constraints in the sigma points and modifies the sigma point that corresponds to the case of constraint violation. Chong [2012] used the UKF for state estimation and showed its ability to estimate uncertain parameters to account for plant-model mismatch. However, in this method, there is no appropriate modification for constraint violation at the sigma point, which may lead to wrong state estimations. Despite the previously mentioned issues, Kalman Filter variants of the state estimators have the nice feature of one-step recursion which is suitable for the online application. Huang [2010] used EKF-NMPC coupling and analyzed robust stability of off-set free output-feedback NMPC using this combination. In contrast to the Kalman Filter methods, constraints in the moving horizon estimation (MHE) method can be handled easily. However, MHE-MPC integration methods may not be suitable for real-time application due to the computational difficulty in solving the nonlinear optimization problem with the same MPC controller update frequency. There are some new methods for addressing faster solution using a simultaneous collocation approach, advanced-step MHE (as-MHE) and sensitivity methods, which are suitable for real-time application to large-scale problems (Zavala *et al.* [2007], Zavala and Biegler [2009b], and Zavala [2010]). Successful coupling of as-MHE-NMPC also has been carried out by Huang [2010] for an air separation unit; despite this, still there is no stability analysis for the as-MHE-NMPC formulation. Recently, Ellis *et al.* [2014b] proposed application of an MHE formulation in the implementation of LEMPC formulation. They also analyzed the closed-loop stability of the output-feedback based LEMPC in the presence of process and measurement noise.

2.2.5 Stability Analysis

Stability analyses for the single-layer method are provided by Angeli *et al.* [2012], Heidarinejad *et al.* [2012a] and Omell and Chmielewski [2013]. Addition of a terminal condition, application of a Lyapunov based model predictive control formulation and implementation of an infinite horizon MPC formulation are some different techniques which have been used for the stability analysis of EMPC in these research works. Also, Ellis and Christofides [2014a] carried out a stability analysis for a two-layer structure of dynamic economic optimization and MPC using a Lyapunov based model predictive control formulation.

2.2.6 Computational Performance Improvement

Different methods such as Fast Nonlinear MPC algorithms for a two-layer structure (Kadam and Marquardt [2004]), advanced-step NMPC and advanced multi-step NMPC for the single-layer structures (Zavala and Biegler [2009a], Yang and Biegler [2013]) have been developed to reduce the computational time of the dynamic optimization problems. Also some other researchers have tried to reduce the computational time by employing the idea of distributed model predictive control (DMPC). For example Chen *et al.* [2012] have applied a distributed Lyapunov based EMPC formulation to a catalytic alkylation of benzene process network. They could show that the average computational time for the solution of optimization problem decreases by half for a standard Lyapunov based EMPC. Process model reduction is another effective method to reduce the computational demand. Time-scale separation strategies could be used to perform the process model reduction. Yu and Biegler [2014] and Tosukhowong *et al.* [2004] introduced different time-scale separation strategies based on the eigenvalue analysis of the linearized process model.

Chapter 3

Formulations and Comparison Methodologies

This chapter presents the single-layer and two-layer formulations used for a systematic comparative performance analysis. Also, the problem solution techniques applied and the assumptions in the implementation of real-time optimization are addressed in the next sections. Moreover, a consistent real-time optimization design is proposed for a fair comparison between the two general approaches. The comparison methodology for the performance evaluation of the selected single- and two-layer formulations is included in the last section of this chapter.

3.1 Single-layer Formulation

As discussed in the literature review, assuming a-priori defined optimal setpoints for the implementation of economically optimal setpoint tracking in the single-level fashion is a common formulation. However, there is no necessity for an a-priori defined setpoint in the general EMPC formulation. An EMPC formulation with a pure economic objective function is used in Chong and Swartz [2013] for a multi-level implementation of the single-layer approach. Thus, their EMPC formulation is not limited to an a-priori known optimal setpoint. An EMPC formulation of equation (3.1) is considered for a representative single layer approach, which is similar to the single-layer formulation in Chong and Swartz [2013] with a pure economic objective function.

$$\begin{aligned}
\underset{U(k)}{\text{maximize}} \quad & \Phi_{eco}(Y(t), u(t), C(t)) \\
\text{subject to} \quad & \dot{X} = F(X(t), u(t); \theta) \\
& Y(t) = X(t) + \hat{d}_i \\
& \hat{d}_i = Y_m - X(t_i|t_{i-1}) \\
& G(Y(t), u(t)) \leq 0 \\
& u(t) = U(k), \;\; t_i + (k-1)T_e \leq t \leq t_i + kT_e, \forall k = 1, ..., N_e \\
& X(t_i) = X(t_i|t_{i-1})
\end{aligned} \tag{3.1}$$

where $Y(t)$, $u(t)$ & $X(t)$ are vectors of output, input and state variables at time t and $U(k)$ is piecewise constant input sequence at discrete time instance k. $C(t)$ represents a sequence of known economic disturbances at the current time and the predicted economic information in the near future. For instance $C(t)$ could be unit price prediction. θ denotes the process model parameters. In this single-layer formulation, it is assumed that all of the output variables are measured. A vector of the prediction bias parameter $\hat{d}_i$ is embedded in the process model to account for the effect of unknown disturbances in the model prediction. The prediction bias is updated based on the prediction error of the $(i-1)$th iteration step of the EMPC. T_e and N_e represent the update time and the economic optimization horizon and $U(k) \in \mathbb{R}^{n_u}$, $\forall k = 1, ..., N_e$ is a sequence of decision variables applied to interval k in the ith EMPC iteration step. The $G(Y(t), u(t))$ constraints include input constraints, output constraints and any other type of desired nonlinear path constraints. Also the last constraint denotes the update of state variables at t_i based on the evolution of states using the process model and the previous state values. In each EMPC iteration step the optimization problem is solved subject to the process model and the constraints $G(Y(t), u(t))$. Then the first input solution $U(1)$ is implemented to the process using a zero-order hold until reaching the next update time (t_{i+1}). After solving the optimization problem of the ith EMPC iteration step, the horizon moves forward and these steps will be repeated until the end of the process operation time.

3.2 Open-loop DRTO-MPC Formulation

The EMPC formulation of equation (3.1) is used for the economic optimization problem in the both two-layer approaches. However, there are some differences in the design of the DRTO layer and the implementation of optimal manipulated variables. The optimization layer in the two-layer approach has a lower update frequency than that of the EMPC formulation. Also, in the EMPC approach the optimal inputs are directly applied to the processes whereas, in the two-layer DRTO-MPC approach the economically optimal inputs and their corresponding outputs are re-sampled with the MPC control layer update time to be used as an optimal setpoint in the standard linear MPC formulation of Equation (3.2) which could be found in Maciejowski [2002]:

$$\begin{aligned}
\underset{U_c(n)}{\text{minimize}} \quad & \Phi_c = \sum_{n=1}^{N_p} ||y(n+1) - R(n+1)||_Q^2 + \sum_{n=1}^{N_c} (||U_c(n) - U_R(n)||_\Gamma^2 + ||\Delta U_c(n)||_S^2) \\
\text{subject to} \quad & x(n+1) = A_e x(n) + B_e U_c(n), \qquad n = 1, ..., N_c \\
& x(n+1) = A_e x(n) + B_e U_c(N_c), \qquad n = N_c + 1, ..., N_p \\
& y(n+1) = C_e x(n+1) + \hat{d}_j \\
& D_e y(n+1) + E_e U_c(n) + F_e \leq 0, \qquad n = 1, ..., N_p \\
& \hat{d}_j = Y_m(t_j) - C_e x(t_j|t_{j-1}), \\
& x(1) = x(t_j|t_{j-1}), \qquad t_j \in [t_i, t_{i+1})
\end{aligned} \tag{3.2}$$

Where T_e, T_c, N_c, N_p, Q, Γ & S are DRTO update time, MPC update time, MPC control horizon, MPC prediction horizon, output weight, input weight and input change penalty weight matrices. $R(n+1)$ and $U_R(n)$ are reference output and input signals which are

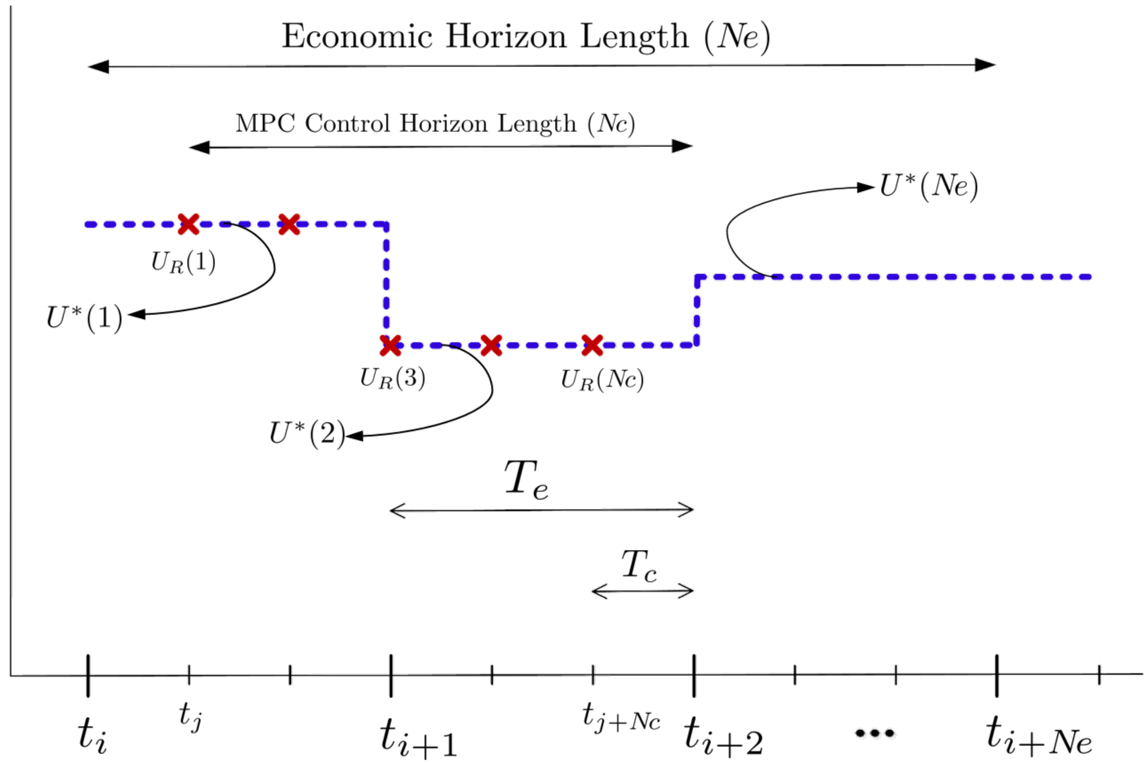

Figure 3.1: Re-sampling of the solution of the economic optimization problem $U^*(k)$ to build the reference input sequence $U_R(n)$ for the MPC problem at $t = t_j$.

calculated in the most recent DRTO iteration step. Figure 3.1 shows the reference input values $U_R(n)$ which result from the re-sampling of the solution of the economic optimization problem $U^*(k)$. In this figure, t_i corresponds to the recent economic solution update $\begin{bmatrix} U^*(1) & U^*(2) & ... & U^*(N_e) \end{bmatrix}$. The index for the solution of the economic optimization problem $U^*(k)$ starts from $k = 1$ for each DRTO iteration step. t_j shows the current MPC update time which starts from $t_j = t_i$ for the first MPC iteration step and increases with the MPC sample time T_c for the next MPC iteration steps in the economic optimization time interval $[t_i, t_{i+1})$. The index of the re-sampled input $U_R(n)$ is from $n = 1$ to $n = N_c$ for each MPC iteration step. Equation 3.3 is used for the reference input re-sampling:

$$U_R(n) = \begin{cases} U^*(1), & 1 \leq n < 1 + (t_{i+1} - t_j)/T_c \\ U^*(k), & 1 + (t_{i+k-1} - t_j)/T_c \leq n < 1 + (t_{i+k} - t_j)/T_c \end{cases}, \quad k = 2, ..., 1 + ceil(\frac{N_c T_c}{T_e}) \quad t_j \in [t_i, t_{i+1}) \tag{3.3}$$

Then, the re-sampled optimal input sequences $U_R(n)$ are used to integrate the same nonlinear process model, which is used in the economic optimization layer of equation (3.1), to obtain the reference output variables $R(n)$. The reference signals must be provided up to the time which is needed by the horizon of the last MPC controller before the next economic layer update time arrives. This time is equal to $t_i + T_e + N_p T_c$. The $ceil(.)$ function in the upper bound of k rounds a real number to the closest upper integer number.

In this MPC formulation A_e, B_e, C_e, D_e, E_e, and F_e in the process model and path constraint result from the linearization in ith update time interval of the economic optimization layer ($[t_i, t_{i+1})$). The original process model and path constraint in the Equation (3.1) are linearized around the average values of the optimal setpoint signals $R(n)$ & $U^*(k)$ at the two ends of the time horizon.

In each MPC step j a bias parameter is updated which is calculated as a difference between the measured output $Y_m(t_j)$ and the predicted output from the $(j-1)$th MPC step (x$(t_j|t_{j-1})$). Also, the last constraint in Equation (3.2) denotes the update of initial state variables based on the evolution of the states from the previous MPC iteration step. It should be noted that the initial state variables are updated based on the measurements, when full states measurements are available.

The first control input vector $U_c(1)$ is implemented to the process using a zero-order hold until reaching the next MPC controller update time t_{j+1}. The MPC iteration steps proceed for all $t_j \in [t_i, t_{i+1})$. After the completion of the full sequence of the MPC steps in interval $[t_i, t_{i+1})$, the economic optimization layer updates the economically optimal reference signal at t_{i+1} for the MPC sequences of the $(i+1)$th time interval (i.e. $[t_{i+1}, t_{i+2})$).

The MPC formulation of equation 3.2 does not include ny kind of stability constraints because it is intended to compare the single-layer and two-layer structure with the simplest possible MPC control approach. This assumption is reasonable for open-loop stable systems and a sufficiently long prediction horizons and could lead to a general performance comparison which is independent of stability constraint effects. However, the MPC formulation of equation 3.2 could be readily replaced by other variants of MPC formulations.

3.3 Closed-loop DRTO-MPC Formulation

In the CL-DRTO-MPC formulation closed-loop control prediction is incorporated in the economic optimization level. In this formulation, similar to the OL-DRTO formulation, economic performance of the processes is optimized subject to the desired input, output and path constraints. In the CL-DRTO-MPC formulation, closed-loop control interaction of the MPC and the available model of the process must be included in a form of closed-loop dynamic constraints in the DRTO layer to moderate undesired effects of the model mismatch between the economic optimization layer and the regulatory control layer. A closed-form solution of a general controller formula could be embedded in the economic optimization problems to account for the closed-loop dynamic behavior of the process. However, due to the bound constraint on the control action and the operational constraints of the process output, there is no explicit solution for the general formulation of the MPC problem. Solution of the necessary and sufficient first-order Karush-Kuhn-Tucker(KKT) optimality conditions is equivalent to the solution of the MPC QP optimization problem. Jamaludin and Swartz [2016] were able to show that it is possible to include a closed-loop prediction of the process systems in the DRTO formulation using the KKT condition.

A multilevel simultaneous solution approach could be used to solve the resulting NLP problem. This approach significantly increases the size of the DRTO problem. However, there is a promising study on the problem reduction of the rigorous inclusion of the closed-loop dynamic prediction in the DRTO approach(Jamaludin and Swartz [2017a]). In this study three methodologies of hybrid formulation, bilevel formulation, and input clipping formulation are used to approximate the closed-loop response prediction.

Unlike the simultaneous solution approach which needs a full discretization of the control inputs and the state variables, in the sequential solution approach only the control inputs are discretized and dynamic constraints are evaluated using ODE solvers. Thus, the sequential approach has a the potential strength to maintain the dynamic optimization problem size small, using the input vector discretization technique. There could be an opportunity to solve CL-DRTO problems more efficiently by reducing the computational effort using a sequential solution strategy. Also, in the implementation of CL-DRTO using simultaneous solution approach, the original multilevel dynamic optimization problem is reformulated as a single-level mathematical program with complementarity constraints (MPCC)(Jamaludin and Swartz [2017b]). The sequential solution approach does not require optimization problem reformulation. Therefore, implementation of CL-DRTO using the sequential solution approach is easier than that of the simultaneous approach. However, the sequential approach has a potential drawback due to derivative discontinuities when MPC input constraints are changed from active to inactive and conversely from inactive to active mode. In the current section a sequential solution framework is developed which is able to directly solve the MPC subproblems in the form of equation 3.2 in the CL-DRTO optimization layer. Therefore, this method reduces the size of the primary optimization problem by the elimination of the KKT optimization constraints and the associated MPC decision variables in the multilevel optimization problem of the CL-DRTO layer. In this sequential approach, solution of multiple QP subproblems, which arise from the MPC iteration steps over the economic optimization horizon, accounts for the closed-loop output prediction in the DRTO level. The QP subproblems must be solved in each function evaluation of the economic optimization problem. A detailed representation of the sequential approach is depicted in a flow-diagram system in figure 3.2. An overview on the flow-diagram could be useful for the basic understanding of the flow of the tasks in the solution of the QP subproblems and the way each subproblem communicates with the other optimization problems and the primary optimization problem.

The initial input sequence of the U^{DRTO} could be obtained from the solution of the previous

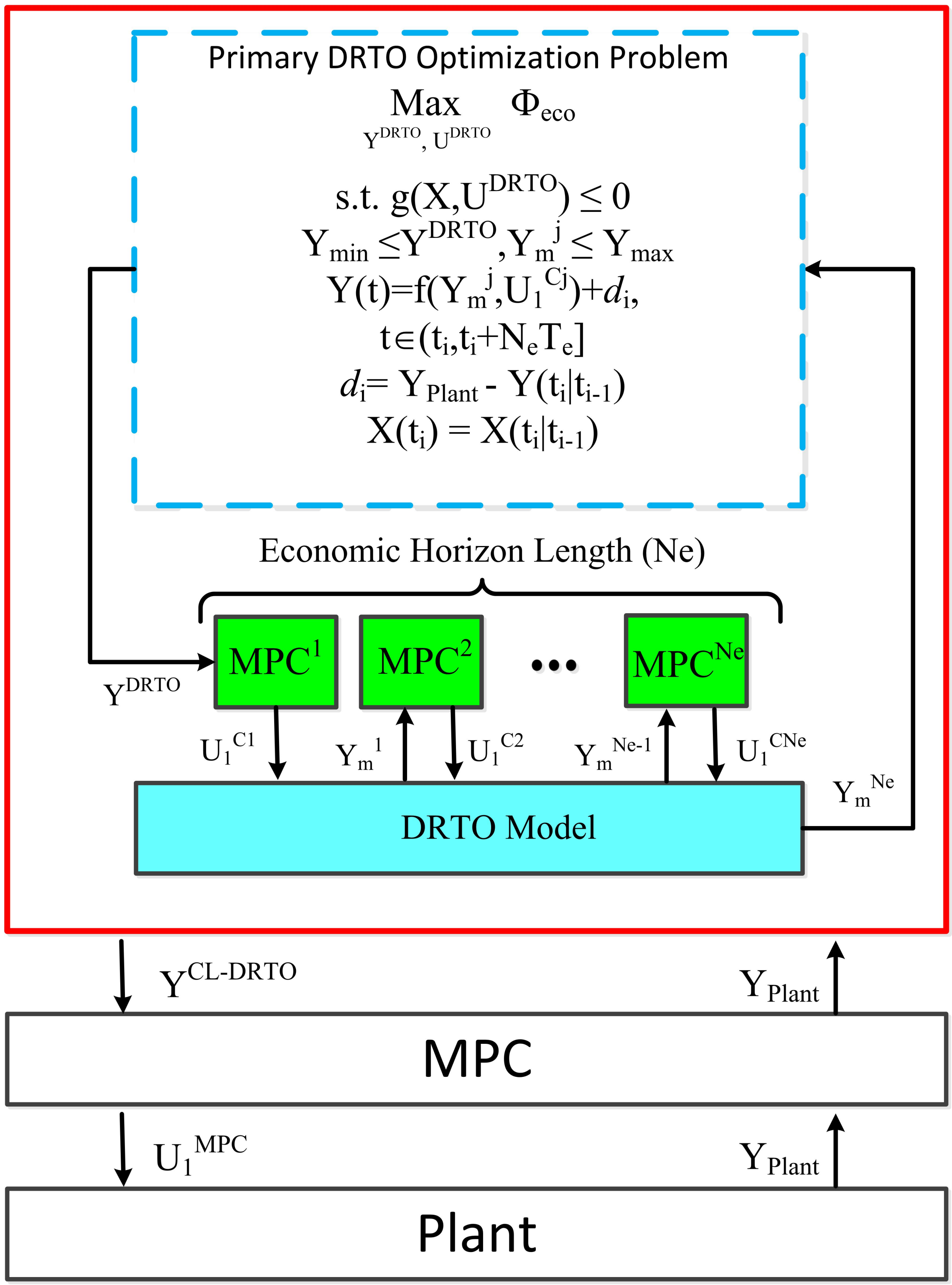

Figure 3.2: A sequential implementation framework for the multilevel optimization problem of the CL-DRTO layer in the two-layer configuration.

CL-DRTO step. Integration of the DRTO process model using the initial input sequence of the previous CL-DRTO step could result the required initial setpoints Y^{DRTO} for the initialization step of the closed-loop economic optimization problem. Figure 3.2 shows the MPC subproblems in the ith DRTO update interval $[t_i, t_{i+1})$. The MPC subproblems MPC^j, & $j \in \{1, ..., \mathrm{N}\}$) must be solved over the entire economic optimization horizon. $N = (T_e/T_c)N_e$ determines the number of the MPC subproblems which are placed in each DRTO update interval. The first control action (U_1^{Cj}) of each MPC^j subproblem in the ith DRTO update time interval is applied to the DRTO model. The resulting hypothetical measured output values (Y_m^j) updates the MPC bias $\hat{d}_j$ in the MPC formulation of equation 3.2. Also, the state values which corresponds to the outputs Y_m^j of the DRTO model are used to initialize the next MPC subproblem (MPC^{j+1}). This pattern is repeated until approaching the end of the economic optimization horizon ($t_i + N_e T_e$). For the last ($N - N_c$) MPC subproblems extra optimal inputs are required after the ending element of U^{DRTO}. Therefore, the extra input setpoints are assumed to be equal to the last element of the optimal input setpoint ($U^{DRTO}(N_e)$). A similar assumption holds for the extra output setpoints of the last ($N - N_p$) MPC subproblems.

After the solution of the sequence of MPC subproblems the hypothetical measured output values Y_m^j are sent to the primary economic optimization problem at the end of each DRTO economic optimization horizon. These values are used for the calculation of the economic objective function Φ_{eco}. The output constraints on Y_m^j could be considered in each individual MPC subproblem. However this could cause feasibility issues for the MPC subproblems. Therefore, the output constraints for the DRTO model outputs Y_m^j, together with the path constraints and input-output constraints for the setpoints, are considered in the economic optimization layer. A feedback of the plant output measurements is provided to the CL-DRTO method in each DRTO update time to update the bias d_i of the DRTO model in each CL-DRTO step. The initial state values of $X(t_i)$ are obtained from the evolution of states $X(t_i|t_{i-1})$ at the previous CL-DRTO step t_{i-1} using the DRTO model. This overview shows a coherent closed-loop formulation scheme that includes the MPC optimization subproblems, virtual process plant included as a DRTO model, primary economic optimization problem and the way these problems are connected to each other in the proposed sequential approach. The primary problem could be solved using an appropriate NLP solver. Details on the relevant assumptions, design parameter specifications and the solution steps are discussed in the next sections.

The communication of the entire block of the CL-DRTO layer formulation in figure 3.2 with the MPC control layer and the actual plant is similar to that of the OL-DRTO. Solution of the CL-DRTO layer, $Y^{CL-DRTO}$ and $U^{CL-DRTO}$ are re-sampled in a similar form of equation 3.3 to provide setpoint for the lower level of MPC controller.

3.4 Real time Optimization Design

The following steps should be considered for the choice of the suitable economic optimization update time, T_e; and the economic optimization horizon, N_e in both single-layer and two layer method; the MPC control layer update time, T_c; the MPC control horizon, N_c and the MPC prediction horizon, N_p in the two-layer approach.

1. **MPC controller update time in the two-layer formualtion:** update time selection is the most straightforward part which exists in the literature (Shridhar and Cooper [1998]). To this end a first-order plus dead-time (FOPDT) process model is determined around the initial operating conditions (Marlin [1995]) to find the input-output time constants (τ_{RS}) and process time delays (θ_{RS}) for process inputs S and outputs R. The process time constants and time delays are used in the following formula to calculate the MPC update time:

$$T_c = Min(Max(0.1\tau_{RS}, 0.5\theta_{RS})) \tag{3.4}$$

2. **MPC control and prediction horizon length in the two-layer formualtion:** As the MPC formulation of equation (3.2) does not have any type of stability constraint and/ or terminal condition to guarantee the stability, the prediction horizon is chosen sufficiently long to insure stability of the MPC controller in the two-layer approach.

Thereafter the control horizon could be chosen according to a methodology such as in Garriga and Soroush [2010]. For open-loop stable and nonsquare multi input-multi output (MIMO) systems, the initial value of the control horizon could be determined from the maximum of the various combinations of $(\tau_{RS} + \theta_{RS})$ for process inputs S and outputs R. The input-output time constants (τ_{RS}) and the corresponding process time delays (θ_{RS}) are calculated from the FOPDT model of the process. They also mention that trial and error could be useful for the final tuning of the control horizon. They state that the horizon should be large enough to extend over all significant adjustments in the manipulated variable required to implement a setpoint change. Without loss of generality it is also considered that the MPC horizon length is less than the horizon of the economic optimization. Otherwise the optimal set point could not be provided for the control layer beyond the horizon of the economic optimization. This assumption will guarantee that the current DRTO iteration step could provide a full length optimal setpoint which is required by the MPC formulation.

3. **EMPC update time:** Considering the discussion in the motivating problem part (section(1.1)), it is assumed that the update time in the single-layer approach could be equal to that of the control layer in the two-layer structure. Hence, MPC sample time is chosen for the EMPC formulation, because EMPC should be able to account for both of the economic optimization and control tasks.

4. **Economic optimization horizon length in the single- and dual-layer methods:** It is shown by Ellis and Christofides [2015] that in some case study problems it is possible to improve the economic performance by increasing the horizon length of the economic optimization problem. Therefore EMPC and/ or the DRTO horizon length could be increased to the point that the economic performance improvement is negligible. The horizon length corresponding to the maximum improvement is selected as the suitable horizon.

5. **DRTO layer update time in the two-layer formulation:** The DRTO layer update time could be bigger than the EMPC update time. The bigger economic optimization update time means that the optimal setpoints are updated less frequently. The slower eco-

nomic update may cause less economic performance improvement in comparison to that of the EMPC for a case of an equal economic optimization horizon. Tosukhowong *et al.*, 2004 proposed a methodology to select the update time in a reasonable range for the DRTO layer. They suggest to calculate the eigenvalues of the linearized process model and sort them from smallest to biggest eigenvalue. Then, the biggest gap of the eigenvalue must be found which could divide the eigenvalues into two groups. Any higher frequency dynamics (i.e. dynamics that are associated with the eigenvalues in the group of the smaller eigenvalues) should be avoided in the selection of the economic layer update time in the dual-layer method. The economic update time could be chosen as $6/(min(group\, of\ bigger\ eigenvalues))$.

3.4.1 Incorporation of Operating Constraints and Objective Function Calculation

According to Zafiriou [1990], the inclusion of hard output constraint in MPC formulation could result infeasible optimization problem and/ or instability in the presence of the unknown disturbances. This problem could happen when there is no available input to move process output to the feasible region in the current MPC iteration step. Therefore, it is important to decide on the appropriate method to incorporate input and output constraints in the MPC control layer of the two-layer methods.

The soft constraint approach penalizes constraint violations in the objective function with a weight parameter to avoid the infeasiblity of the QP optimization problems. The following formulation explains how it is possible to convert a linear inequality hard constraint to a soft constraint by adding a positive slack variable ϵ in a general optimization problem:

$$\alpha_{min} - \epsilon \leq CX \leq \alpha_{max} + \epsilon. \tag{3.5}$$

where C is a row vector with the same size of the general decision variables X and α_{min} & α_{max} are inequality bounds. A penalty term of the form $w\epsilon^2$ must be added to the objective function where w represents constraint violation weight. This weight must be large enough to prevent constraint violation when the original optimization problem with the hard constraint is still feasible.

In this work, hard input constraints are handled within the economic layer and control layer in the two-layer approaches. These input constraints are treated in the same way in the single layer formulation. Also, hard output constraints are handled directly in the EMPC formulation and within the economic layer in the two-layer approaches. However, the soft constraint formulation approach is used for output constraint handling in the MPC control layer in the two-layer approaches to account for the infeasiblity issues of the QP optimization problems.

3.4.2 Dynamic Model Evaluation and Optimization Problem Solution

In each iteration step of the DRTO and single-layer formulations a dynamic optimization problem must be solved. Sequential and simultaneous methods are two general strategies to solve dynamic optimization problems. In the sequential method only control variables are discretized. In this strategy model integration is required in each function evaluation. In this study both of the single layer and two-layer approaches are implemented using a sequential problem formulation. Thus, the process model must be integrated in each function evaluation in the resulting nonlinear programming (NLP) problem. The ODE models in the economic optimization problems are integrated using the ode45 MATLAB built-in solver. The MPC optimization subproblems in the CL-DRTO formulation and the MPC control layer problems are solved using the quadprog QP solver with the interior-point algorithm. The NLP problems which result from the economic optimization problem are solved using the fmincon NLP solver with the interior point algorithm.

3.5 Comparison Methodology

The first case study problem is considered to evaluate the performance of selected single- and two-layer formulations in the presence of different unknown disturbance scenarios. Performance evaluation of the selected formulations is conducted for the case of dynamic transitions between operating conditions in the second case study. It is important to operate a process with minimal operating and safety constraint violations and to achieve enhanced economic performance using a modest computational effort. Therefore, the following criteria are considered to tabulate performance results for the purpose of comparison in the presence of different operating condition scenarios:

3.5.1 Comparison Criteria

1. **Net profit:**

   As mentioned in the previous sections, optimal process operation is the main purpose of the application of RTO methods. In general, the goal of the economic optimization layer could be expressed in different forms of maximizing reaction rate, yield, selectivity, revenue, profit and many other possible desired metrics (Ellis *et al.* [2014a]). However, an economic objective function, which could directly represent economic performance improvement in terms of profit, could explicitly show the economic advantage of one method over the others. This reason encourages us to choose net profit (P) over a fixed simulation time as a criterion to judge the performance of different RTO approaches. This quantity would be calculated using the manipulated inputs and predicted output variables, and the estimated state variables if the full state measurements are not available.

2. **Average run time (ART):**

   There are different approaches to indicate computational effort for the on-line optimization methods such as computation time and problem size. In this study problem, size and number of the required NLP and QP problems for a fixed simulation time may vary in the implementation of different approaches. This different number and size of the NLP and QP are direct consequences of different update times in each formulation and distinct formulation structure for the EMPC, OL-DRTO-MPC and CL-DRTO-MPC formulations. Different size and number of NLP and QP problems in each formulation do not provide a comprehensive overview of the information for the comparison of the computational performance of the selected scenarios. Therefore, it is more preferable to report the ART over the biggest update time intervals among different formulations, to indicate total computational effort which is required in an equal time interval.

The solution time for each individual iteration step of the economic optimization layer in the two-layer formulations and/ or the EMPC formulation are recorded until the end of the simulation time. Then summation of these solution times is divided by the number of DRTO problems that fits into the entire simulation time. A similar procedure is carried out to obtain the solution time for QP problems of the MPC control layer. The value of ART criteria is the average solution time of the economic optimization problem for the single-layer method and the summation of the average solution time of the economic optimization and MPC problems for the dual-layer methods.

3. **Cumulative output constraint violation (COCV):**

   Operating a process system within the predefined constraints could maintain the effectiveness of process design, specified product qualities and safety of the process. Thus, it is important to satisfy these constraints and/ or to reduce constraint violation in the cases where the constraint violation is unavoidable. Qualitative constraint violation comparison of single- and two-layer methods could clarify the severity of the constraint violation where there is a significant difference in the constraint violation results, although it does not provide a conclusive result on the amount of the constraint violation in the entire simulation time interval. A COCV criteria of equation 3.6 is developed to account for the constraint violation of each individual constraint. The COCV metric could be helpful to conduct a systematic comparison of the capability of each formulation to maintain process operation within the predefined constraints.

$$COCV = \int_{t_0}^{t_f} \Big((\alpha_{min} - CX)R^{LB} + (CX - \alpha_{max})R^{UB}\Big)\, dt,$$
$$R^{LB}(X) = \begin{cases} 0, & CX \geq \alpha_{min} \\ 1, & CX < \alpha_{min} \end{cases}, \tag{3.6}$$
$$R^{UB}(X) = \begin{cases} 0, & CX \leq \alpha_{max} \\ 1, & CX > \alpha_{max} \end{cases}.$$

where the COCV accounts for the inequality constraint violation of equation (3.5) and R^{LB}, R^{UB} are switch functions for the lower and upper bound constraint violation. The COCV integration could be numerically calculated using trapezoidal method for the numerical values of the variable X.

3.6 Chapter Summary

In this chapter a detailed discussion on the problem formulations and the implementation method, appropriate design assumptions and the comparison criteria for the purpose of a systematic and fair performance comparison are included. Also a detailed overview on the sequential solution framework for the implementation of the CL-DRTO formulation is presented. The next chapter focuses on the performance comparison of the selected economic optimization formulations in the presence of unknown disturbances for the first case study problem.

Chapter 4

First Case Study Problem

4.1 Case Study Process: Two CSTRs in Series

In this chapter there is a brief description of the case study process. The process description is followed by process modeling, operational constraints, explanation on the different sources of disturbances, and the economic objective of the optimal process operation. Also necessary assumptions in the implementation of the online economic optimization methods are included in the related sections. Thereafter, the performance of the chosen single- and two-layer methods are interpreted and compared using the performance criteria.

4.1.1 Process Description

This process was originally considered by Loeblein and Perkins [1998] for the economic analysis of RTO considering model parameter and structural uncertainties. The process consists of two continuous stirred tank reactors (CSTRs) in series with a mixer in between, where an intermediate feed is added, as shown in figure 4.1. Two exothermic and irreversible first order reactions $A \longrightarrow B \longrightarrow C$ take place in both CSTR reactors. The intermediate product B is desired and the final product C is undesired. Pure component A is introduced to the first reactor and the mixer. Cooling is provided to prevent the thermal runaway of the reactors.

4.1.2 Process Modeling and Operational Constraints

It is assumed that volumetric holdup in the reactors is constant. Therefore process dynamics are described by the equations of component mass and energy balances of the reactors. It is also assumed that the mixing process is fast. Therefore accumulation terms in the mixer total mass balance, component mass balance and energy balance are neglected. It is assumed that fluid density, ρ, remains constant during the reaction and mixing processes. Component heat capacities are also constant and equal to c_p. The kinetic coefficients of the two reactions, $k_i(T)$, are Arrhenius type functions. With this set of assumptions, the following model equations for a CSTR could be obtained:

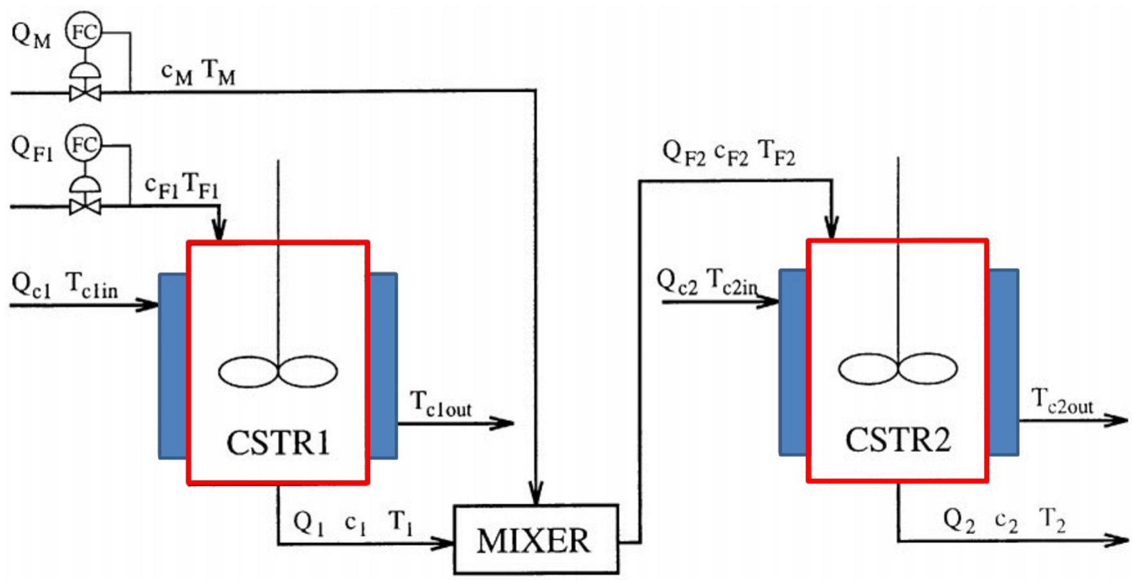

Figure 4.1: Two CSTRs in series with an intermediate feed.

- Overall mass balance equations in terms of volumetric flow rates, Q_{Fi}:

$$0 = Q_{Fi} - Q_i, \qquad i = 1, 2. \tag{4.1}$$

- Component mass balance equations in terms of feed concentrations, $C_{A,Fi}$, $C_{B,Fi}$, $C_{C,Fi}$ and constant reactor holdup, V_i:

$$\begin{aligned}
\frac{dC_{Ai}}{dt} &= \frac{Q_{Fi}}{V_i}C_{A,Fi} - \frac{Q_i}{V_i}C_{Ai} - C_{Ai}k_{0,I}exp(-\frac{E_I}{RT_i}),\\
\frac{dC_{Bi}}{dt} &= \frac{Q_{Fi}}{V_i}C_{B,Fi} - \frac{Q_i}{V_i}C_{Bi} + C_{Ai}k_{0,I}exp(-\frac{E_I}{RT_i}) - C_{Bi}k_{0,II}exp(-\frac{E_{II}}{RT_i}),\\
\frac{dC_{Ci}}{dt} &= \frac{Q_{Fi}}{V_i}C_{C,Fi} - \frac{Q_i}{V_i}C_{Ci} + C_{Bi}k_{0,II}exp(-\frac{E_{II}}{RT_i}), \qquad i = 1, 2.
\end{aligned} \tag{4.2}$$

- Energy balance equations:

$$\frac{dT_i}{dt} = \frac{Q_{Fi}}{V_i}T_{Fi} - \frac{Q_i}{V_i}T_i - \frac{\Delta H_{R,I}}{\rho c_p}C_{Ai}k_{0,I}exp(-\frac{E_I}{RT_i}) - \frac{\Delta H_{R,II}}{\rho c_p}C_{Bi}k_{0,II}exp(-\frac{E_{II}}{RT_i})$$
$$- \frac{q_{cool,i}}{V_i}, \qquad i = 1, 2. \tag{4.3}$$

- The cooling rate, q_{cool} , is a function of the overall heat transfer coefficient,U, the heat exchanger area, A, and the logarithmic mean temperature difference between the cooling water and the reactor temperature:

$$\begin{aligned} q_{cool,i} &= \frac{U_i A_i}{\rho c_p}\Delta T_{ln,i} = U_{ai}\Delta T_{ln,i}, \\ \Delta T_{ln,i} &= \frac{T_{c_{out},i} - T_{c_{in},i}}{ln(T_i - T_{c_{in},i})/(T_i - T_{c_{out},i})}, \qquad i = 1, 2. \end{aligned} \tag{4.4}$$

- The cooling water outlet temperature is determined from the energy balance of the cooling water:

$$q_{cool,i} = Q_{c,i}(T_{c_{out},i} - T_{c_{in},i}), \qquad i = 1, 2. \tag{4.5}$$

In this process model, it is possible to eliminate $T_{c_{out},i}$ in equation (4.5) using equations (4.4):

$$\begin{aligned} q_{cool,i} &= \Lambda_i Q_{c,i}(T_i - T_{c_{in},i}), \\ \Lambda_i &= 1 - exp(-\frac{U_{ai}}{Q_{c,i}}), \qquad i = 1, 2. \end{aligned} \tag{4.6}$$

Substitution of equation (4.6) converts the resulting set of differential-algebraic equation (DAE) process model to a set of ordinary differential equations (ODEs). Therefore the process model could be directly integrated using a general ODE solver in MATLAB. Also the coolant outlet temperature is not an independent state variable. The value of the $T_{c_{out},i}$ can be determined using equations (4.5) and (4.6):

$$T_{c_{out},i} = \Lambda_i T_i + (1 - \Lambda_i)T_{c_{in},i}, \qquad i = 1, 2. \tag{4.7}$$

The steady-state balance equations for the mixer are given below:

- Overall mass balance equation:

$$Q_{F2} = Q_1 + Q_M. \tag{4.8}$$

- Component mass balance equations:

$$Q_{F2}C_{j,F2} = Q_1 C_{j,1} + Q_M C_{j,M}, \qquad j = A, B, C. \tag{4.9}$$

- Energy balance equation:

$$Q_{F2}T_{F2} = Q_1 T_1 + Q_M T_M. \tag{4.10}$$

In total, the model has 8 ODEs, the same number of independent state variables which are reactor temperatures and concentrations, 22 parameters 2 output variables which are T_1 and $T_{c_{out},2}$, and 2 manipulated variables which are feed flow rates, Q_{F1} and Q_M. The nominal operating conditions and parameter values are given in table (4.1).

There are some operation and safety constraints as well as product specifications that limit the admissible operational region of the process. These constraints are mentioned in the following list:

1. *Safety restrictions.* The temperature in both of the reactors should not exceed 350 K.

$$T_1 \leq 350\ K, \qquad T_2 \leq 350\ K. \tag{4.11}$$

2. *Feed supply limitation.* Maximum available total feed flow rate is 0.8 m^3/s.

$$Q_{F1} + Q_M \leq 0.8\ m^3/s. \tag{4.12}$$

Table 4.1: Parameters and nominal operating conditions of the case study process

Variables	Values	
Reactor volumes (m^3)	$V_1 = 5.0$	$V_2 = 5.0$
Feed concentrations ($kmol/m^3$)	$C_{A,F1} = 20.0$	$C_{A,M} = 20.0$
for $i = B, C$ and	$j = F1, M$	$C_{i,j} = 0.0$
Kinetic rate constants (s^{-1})	$k_{0,I} = 2.7 \times 10^8$	$k_{0,II} = 160$
Feed temperatures (K)	$T_{F1} = 300.0$	$T_M = 300.0$
Activation energies (K)	$E_I/R = 6000.0$	$E_{II}/R = 4500.0$
Heat of reactions ($m^3K/kmol$)	$\Delta H_{R,I}/(\rho c_p) = -5.0$	$\Delta H_{R,II}/(\rho c_p) = -5.0$
Cooling water flow rates ($m^/s$)	$Q_{c,1} = 0.7$	$Q_{c,2} = 0.7$
Inlet coolant temperatures (K)	$T_{c_{in},1} = 300.0$	$T_{c_{in},2} = 275.0$
Heat transfer coefficients (m^3/s)	$U_{a1} = 0.35$	$U_{a2} = 0.35$
Nominal operating condition		
Feed flow rates (m^3/s)	$Q_{F1} = 0.274$	$Q_M = 0.236$

3. *Process limitations.* The cooling rate for the available coolant flow rate, Qc, i, with inlet temperature, $T_{c_{in},i}$, is restricted such that coolant outlet temperature should not exceed an a-priori defined temperature. Also there is a minimum feed flow rate required for both feed streams.

$$\begin{aligned} T_{c1out} &\leq 330\ K \\ T_{c2out} &\leq 300\ K \\ Q_{F1} &\geq 0.05\ m^3/s \\ Q_M &\geq 0.05\ m^3/s. \end{aligned} \tag{4.13}$$

4. *Product specifications.* In the second reactor final product outlet should have a raw material concentration less than 0.3 $kmol/m^3$.

$$C_{A,2} \leq 0.3\ kmol/m^3. \tag{4.14}$$

4.1.3 Disturbances and Parameter Uncertainties

Two different types of process and economic disturbances exist in the real-time economic optimization of processes. According to Tosukhowong *et al.* [2004] most economic related changes in the process plants have a low frequency nature. Therefore it is important to differentiate between economic and process disturbances. This is due to the fact that economic disturbances are usually in the sustained signal form and they have lower frequency of change, while process disturbances could exist in both of the sustained and short-term pulse forms.

Feedstock concentrations, $C_{A,F1}$ & $C_{A,M}$, and coolant flow rates, $Q_{c,i}$ could be considered as process disturbance d in the state space process model. Depending on the nature of the changes in the feed source, two different forms of sustained and short-term pulse disturbances are considered. For instance if we have to dissolve and/ or dilute reactant uniformly before feeding it to the reactors, pulse fluctuations may appear in $C_{A,F1}$ and $C_{A,M}$. Also a change in the feed storage source can cause sustained disturbance. These types of the process disturbances could be either known or unknown.

Unit prices of the feedstock, w_{F1} & w_M; and the product, w_B; utility and processing costs, w_{U1} & w_{U2} could be considered as economic disturbances. These types of disturbances are assumed to be known at least for the near future. These economic disturbances could also exist in the forms of sustained and short-term pulses. In this study, it is assumed that the economic disturbances predictions are fixed in a short- and long term future.

Loeblein and Perkins [1998] considered feedstock temperatures, T_{F1} & T_M; heat transfer coefficients, U_{ai}; and side reaction kinetic rate constant, $k_{0,II}$, as uncertain process parameters. However, in our study of the single-layer and two-layer formulation performance comparison, it is assumed that the exact values of these model parameters are known. The uncertainty in these parameters could be considered to study uncertainty effects in the performance evaluation of the single-layer and two-layer methods. It is clear that the uncertainty in the above mentioned parameters could be treated as sustained unknown disturbances which start from the beginning of the simulation time. Table (4.2) represents a summary of unknown process disturbances which are considered in the different process model parameters. Moreover, these disturbance scenarios possess various magnitudes, durations, and directions.

Table 4.2: Selected unknown process disturbance scenarios

Duration	Source	Direction	Magnitude
Short-term	Coolant flow rate	Positive pulse	25 %
Short-term	Coolant flow rate	Negative pulse	25 %
Short-term	Fresh feed concentration	Negative pulse	95 %
Sustained	Coolant flow rate	Positive pulse	25 %

4.1.4 Economic Objective

The objective of the optimal process operation is the maximization of the net profit. The net profit rate for this process is defined as the difference between the product value and the costs for raw material and utilities. Nominal values of the cost coefficients are reported in table (4.3), and the economic objective function has the following form:

$$\Phi_{eco} = w_B\Big(V_1C_{B,1} + V_2C_{B,2}\Big)\Big|_{t=t_f} - w_B\Big(V_1C_{B,1} + V_2C_{B,2}\Big)\Big|_{t=t_i} + \int_{t_i}^{t_f}\Big(w_BQ_2C_{B,2} - w_{U1}q_{cool,1} - w_{U2}q_{cool,2} - w_{F1}Q_{F1} - w_MQ_M\Big)\,dt. \tag{4.15}$$

where the final time is defined in terms of economic optimization horizon and update time ($t_f = t_i + N_eT_e$). The first term in equation (4.15) shows the difference between final and initial asset value of the product B inside the reactors. The second term of the economic objective function represents the revenue of the product B in the outlet flow of the second reactor. The product asset value and revenue should be maximized which means that a lower amount of raw material would be wasted in the form of unreacted and undesired components in the outlet flow of the process. The remaining terms are the cost of cooling rate in the utility system of the first and second reactors and the cost of inlet raw material flows. The total utility and raw material cost should be minimized to improve the net profit.

It is assumed that the measurements of the variables are available for the calculation of the objective function. It should be remarked that in some cases unknown disturbances appear explicitly in the objective function and there is no alternative form for the calculation of objective function. Therefore, unknown disturbance must be estimated for the calculation of the economic objective function (See Ochoa *et al.* [2010]). An unknown disturbance effect which is in the form of a linear combination with the available information in the objective function, has no effect to the solution of the economic optimization problem. Thus, disturbance estimation is not required for this special form of the objective function (See Amrit *et al.* [2013]).

Table 4.3: Nominal values of the cost coefficients

Variables	Values	
Nominal unit prices	$w_B = 10.0$	$(£/kmol)$
$w_{U1} = 0.01$	$w_{U2} = 1.0$	$(£/(m^3K))$
$w_{F1} = 0.1$	$w_M = 0.1$	$(£/m^3)$

The final condition in the economic objective function of equation (4.15) means that it is also desired to maximize product B concentration inside the reactors at the end of each dynamic optimization horizon in the RTO problem. This term is considered in the objective function due to the fact that reaching the end of the horizon in each RTO step does not mean the process operation is terminated. This final condition could prevent large input actions at the end of economic optimization horizon for the continuous time processes. Therefore, this final term is needed to keep the product concentration in its highest possible value for the next RTO steps. The optimal steady state process condition with respect to the economic objective function and operating constraints is reported in Loeblein and Perkins

[1998] for the set of nominal model parameters and the cost coefficients in tables (4.1) and (4.3). The nominal operating conditions are such that the first reactor should work at the maximum temperature and the second reactor should work under the maximum cooling for the economic optimal operation. Therefore, the maximum acceptable temperature in the first reactor, $T_1 = 350\ K$ and the maximum effective cooling water outlet temperature of the second reactor, $T_{c2out} = 300\ K$ are active constraints. Thus, plotting the dynamic behavior of these two state variables could provide important insight in our comparison study.

Nevertheless, there is no guarantee that regulating the system at these active constraints could necessarily result an optimal economic performance in the presence of the unknown disturbance scenarios in this particular example. There are the following possibilities which cause a deterioration in performance by the active constraint regulation method:

1. The active constraints might not be reachable predefined setpoints due to the limitations on the manipulating input variables in the presence of unknown short-term and/ or sustained disturbances and the model uncertainty.

2. In the presence of the unknown process disturbances and the model uncertainty regulating the system at the fixed optimal output setpoints would demand for different manipulating variables, Q_{F1} & Q_M. Amrit *et al.* [2013] assume that there is an a-priori known optimal steady-state setpoint in their case study problem. They showed that economic optimizing approaches with a pure economic, regulatory, and hybrid objective function could result different setpoint tracking, constraint violations, and economic performance. While, the fixed a-priori known setpoint may not be true optimal value in the presence of unknown disturbances and model uncertainty.

3. Optimal process operation on the boundary of the admissible operating region could potentially increase the possibility of constraint violations in the presence of the unknown disturbances and uncertainties. This could be a serious issue if it happens for the safety constraints. Tosukhowong *et al.* [2004] showed that steady state RTO (SS-RTO) could cause constraint violation in the operating condition transition and in the presence of

unknown disturbances and model parameter changes. Also they could show that using the steady state model in the RTO level would result lower economic improvement in comparison with the DRTO methods. As opposed to the SS-RTO, the DRTO methods use a dynamic process model could enable them to predict the dynamic behavior of the output in addition to the steady state condition. This capability could moderate the undesired constraint violation effects.

Considering the above explanation on the possible issues of using regulatory controller and SS-RTO to account for the unknown disturbance effects on the economic and stabilization performance of optimal process operation, this case study focuses on the performance comparison of the EMPC formulation with the two-layer DRTO structures which are mentioned in the sections (3.1), (3.2) and (3.3) of the previous chapter.

Implementation results for the EMPC, OL-DRTO-MPC and CL-DRTO-MPC formulations in the presence of the unknown disturbance scenarios of table (4.2) are discussed in the next section.

4.2 Results and Discussion

EMPC, OL-DRTO-MPC and CL-DRTO-MPC approaches are implemented in the presence of the chosen unknown disturbance scenarios of table (4.2). In all of the scenarios a pulse change occurs at $t = 30s$. The pulse width of $30s$ and/ or $90s$ is considered which corresponds to the duration of the short-term and sustained disturbance cases. The optimal profit, average run time and constraint violations that are discussed in the previous chapter, are reported for each scenario. The resulting trends of changes and dynamic behavior of the outputs and their corresponding input actions are depicted and discussed for each formulation. In the performance comparison section, the comparison criteria are tabulated and discussed according to the available results in the literature and the expectations for each disturbance scenario.

4.2.1 Single-layer EMPC Implementation

The EMPC formulation of equation (3.1) is used for the optimal operation of the process with the design parameters of table (4.4). According to the guidelines of section (3.4) in the previous chapter, a small update time of $T_e = 5s$ is chosen to perform the economic optimization and the regulation tasks in the EMPC formulation. Also, a larger update time period of $T_e = 30s$ is chosen using the design guidelines of the DRTO layer update time in the dual-layer method in section (3.4) to consider the real-time economic optimization task and to show the necessity of the regulatory control layer for the slower update frequency. In the case of the larger update time, it is expected to observe a higher constraint violation for some of the chosen disturbance scenarios. However, the economic performance improvement may not be diminished significantly by using a slower EMPC update frequency (Tosukhowong *et al.* [2004]).

Table 4.4: EMPC design parameters and the associated NLP size and iteration steps for $t_f = 180s$

$T_e(s)$	N_e	N_{NLP}	N_{Iter}
5	12	24	36
30	2	4	6

An economic optimization horizon length of $h_e = 60s$ is selected. The horizon size (N_e), NLP problem size (N_{NLP}) for each EMPC iteration step and total number of EMPC iteration steps N_{Iter} in the simulation time span are determined, considering the length of the simulation time interval, the two update time cases, and the number of manipulated inputs (Q_{F1} and Q_M). The N_e, N_{NLP} and N_{Iter} are reported in table (4.4). These EMPC problem specifications are common for all of the unknown disturbance scenarios. The N_{NLP} and N_{Iter} could provide an insight for the expected magnitude of the average solution time of each formulation comparing to the other single- and two-layer formulations. The interior-point algorithm in MATLAB fmincon solver is used to solve the resulting NLP problems in both of the single- and two-layer formulations. This method has a polynomial computational complexity that shows the solution run-time increases with an increase in the problem size N_{NLP} (Ye and Tse [1989] and Papadimitriou [2003]). Therefore, a smaller ART is expected for the smaller N_{NLP}. Also fewer EMPC iteration steps (N_{Iter}) are required to cover a certain simulation time span.

Simulation results of figures 4.2-4.5 show dynamic behavior of the concentration and temperature in the process and the optimal inputs for the chosen disturbance scenarios for the smaller update time. Figures 4.6-4.9 show similar results for the larger update time. The trends of changes, dynamic behavior and the performance of the EMPC are discussed in the performance comparison of section 4.2.4 in the current chapter.

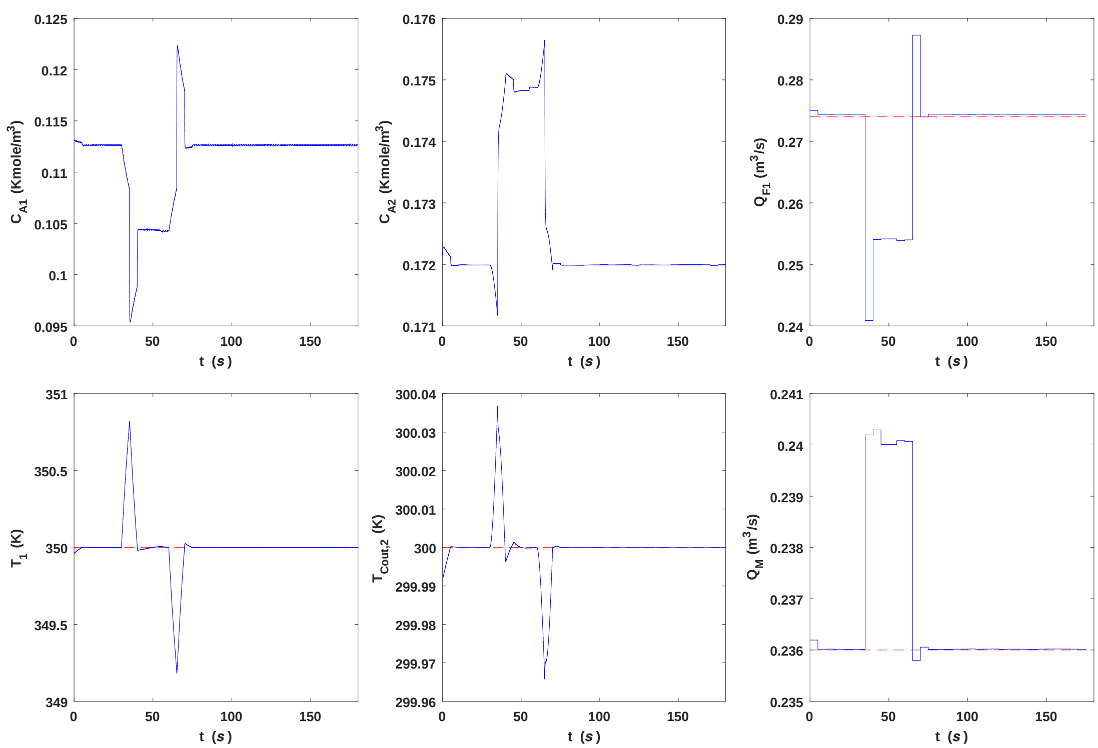

Figure 4.2: Dynamic behavior of the in-series CSTRs for the EMPC optimal process operation ($T_e = 5s$ & -25% short-term pulse disturbance in $Q_{c,1}$). The output and input variables (——) and the output constraints and optimal steady-state inputs (- - -).

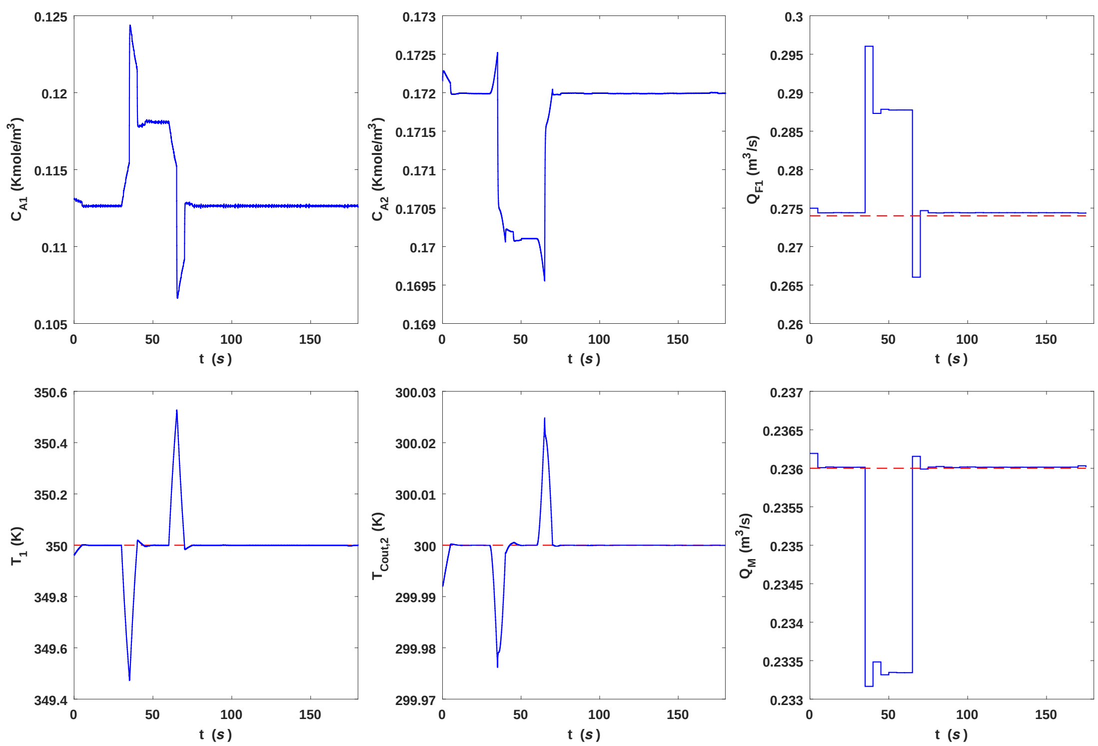

Figure 4.3: Dynamic behavior of the in-series CSTRs for the EMPC optimal process operation ($T_e = 5s$ & $+25\%$ short-term pulse disturbance in $Q_{c,1}$). The output and input variables (——) and the output constraints and optimal steady-state inputs (- - -).

4.2.2 Two-layer OL-DRTO-MPC Implementation

The cascade structure of the economic optimization layer and the MPC control layer, which is described in chapter 3, is implemented with the design and tuning parameters of table (4.5). The economic optimization layer update time is equal to the larger update time of the EMPC and the MPC layer update time is equal to that of the smaller update time in the EMPC implementations. As explained in the formulation and design of the real-time optimization in the previous chapter, the chosen update time for the open-loop two-layer approach would help to conduct a fair comparison of the economic improvement and the regulation performance in the single- and two-layer approaches. The MPC horizon

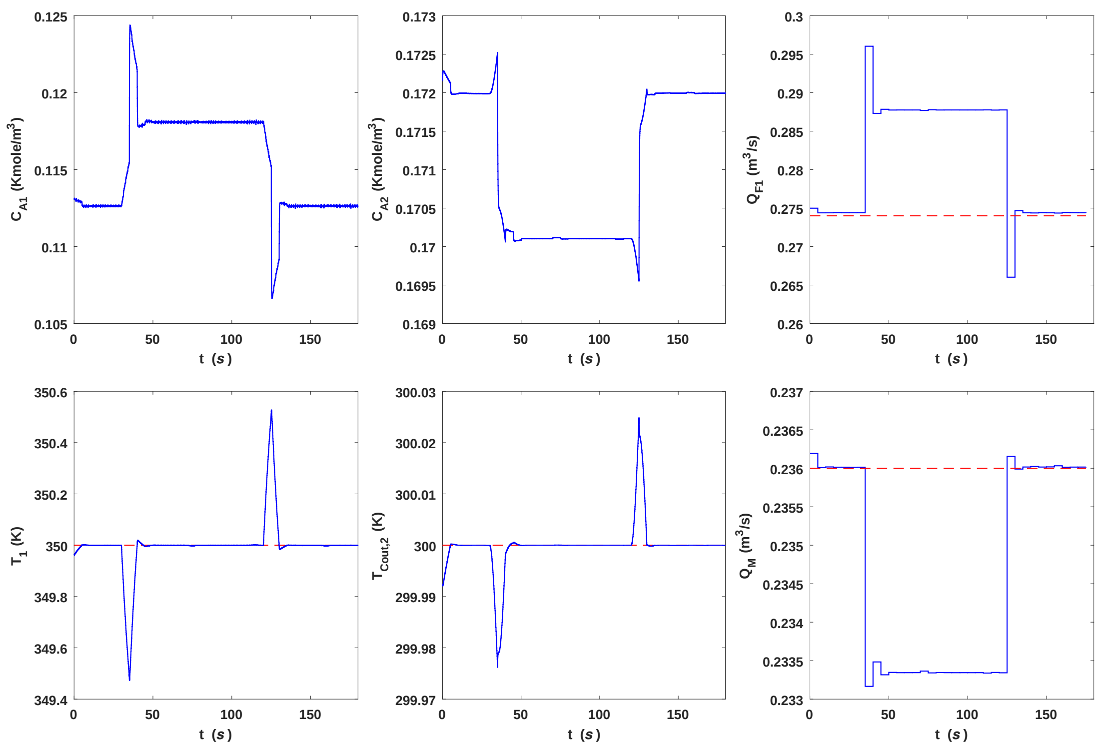

Figure 4.4: Dynamic behavior of the in-series CSTRs for the EMPC optimal process operation ($T_e = 5s$ & +25% sustained pulse disturbance in $Q_{c,1}$). The output and input variables (——) and the output constraints and optimal steady-state inputs (- - -).

is $h_c = 30s$ which is equal to the length of the upper layer update interval. This horizon length leads to the QP problem size of $N_{QP} = 12$. The NLP and the QP problem size and the number of their required iteration steps for the entire simulation time are determined (see table (4.5)) with the same procedure that is used for the previous section. These values could be helpful to justify the computational performance results for the OL-DRTO-MPC formulation. The output constraints in the MPC layer are implemented in the form of the soft constraint formulation to avoid an infeasible QP problem. In table (4.5) $w_c = 10^6$ is the tuning weight for the soft constraint implementation of the output variables in the MPC control layer.

Figures 4.10-4.13 show the simulation results for the chosen disturbance scenarios. Trends

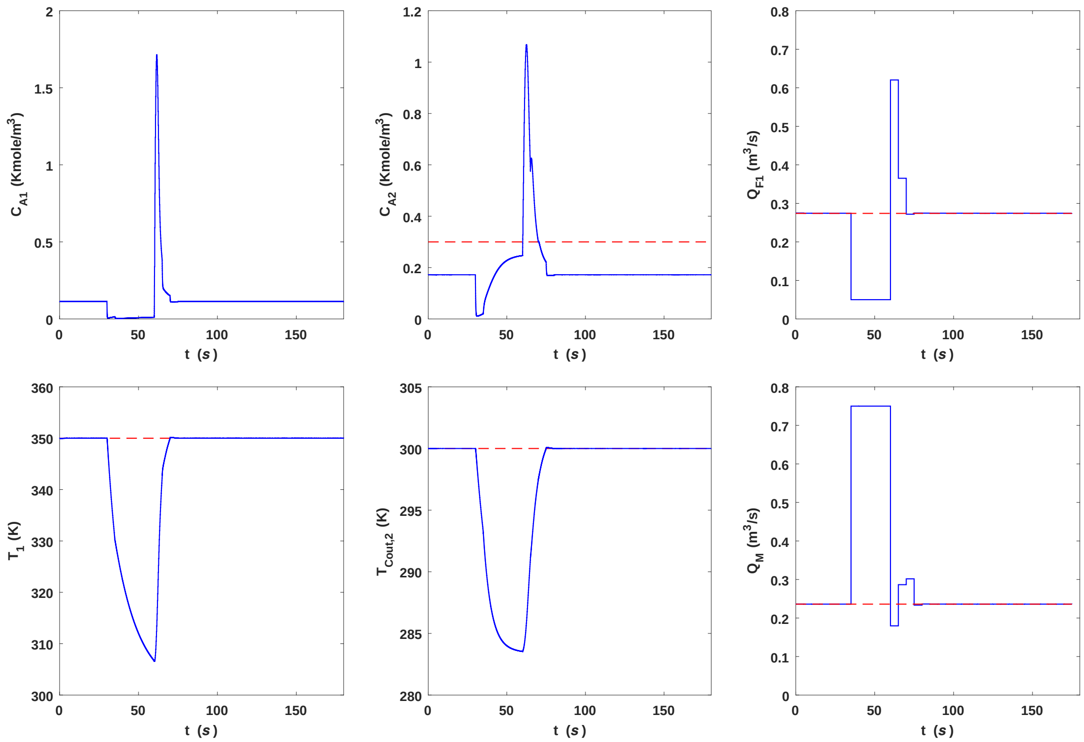

Figure 4.5: Dynamic behavior of the in-series CSTRs for the EMPC optimal process operation ($T_e = 5s$ & -95% short-term pulse disturbance in $C_{A,F1}$ and $C_{A,M}$). The output and input variables (——) and the output constraints and optimal steady-state inputs (- - -).

Table 4.5: OL-DRTO-MPC design parameters and associated NLP & QP sizes and number of their iteration steps for $t_f = 180s$

Automation level	Parameters		Problem sizes & iteration steps	
OL-DRTO	$T_e = 30s$	$N_e = 2$	$N_{NLP} = 4$	$N_{Iter} = 6$
MPC	$T_c = 5s$ $Q = I_{2\times2}$ $S = 0.01I_{2\times2}$	$N_c = 6$ $\Gamma = 0_{2\times2}$ $w_c = 10^6$	$N_{QP} = 12$	$N_{Iter} = 36$

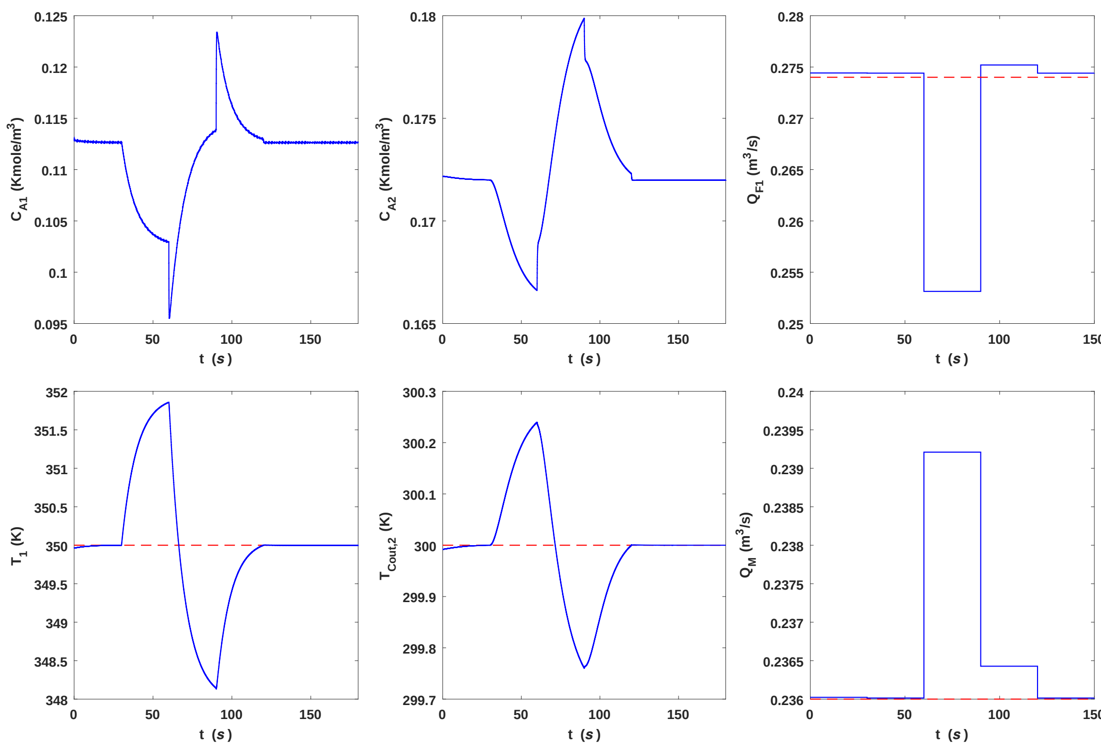

Figure 4.6: Dynamic behavior of the in-series CSTRs for the EMPC optimal process operation ($T_e = 30s$ & -25% short-term pulse disturbance in $Q_{c,1}$). The output and input variables (——) and the output constraints and optimal steady-state inputs (- - -).

of the changes and dynamic behavior of the outputs and the performance of the OL-DRTO-MPC are discussed in the performance comparison of section 4.2.4 in this chapter.

4.2.3 Two-layer CL-DRTO-MPC Implementation

The CL-DRTO formulation of figure 3.2 is implemented in the economic layer of the DRTO-MPC cascade structure. The design and tuning parameters are reported in table (4.6) which are similar to those of the OL-DRTO-MPC formulation.

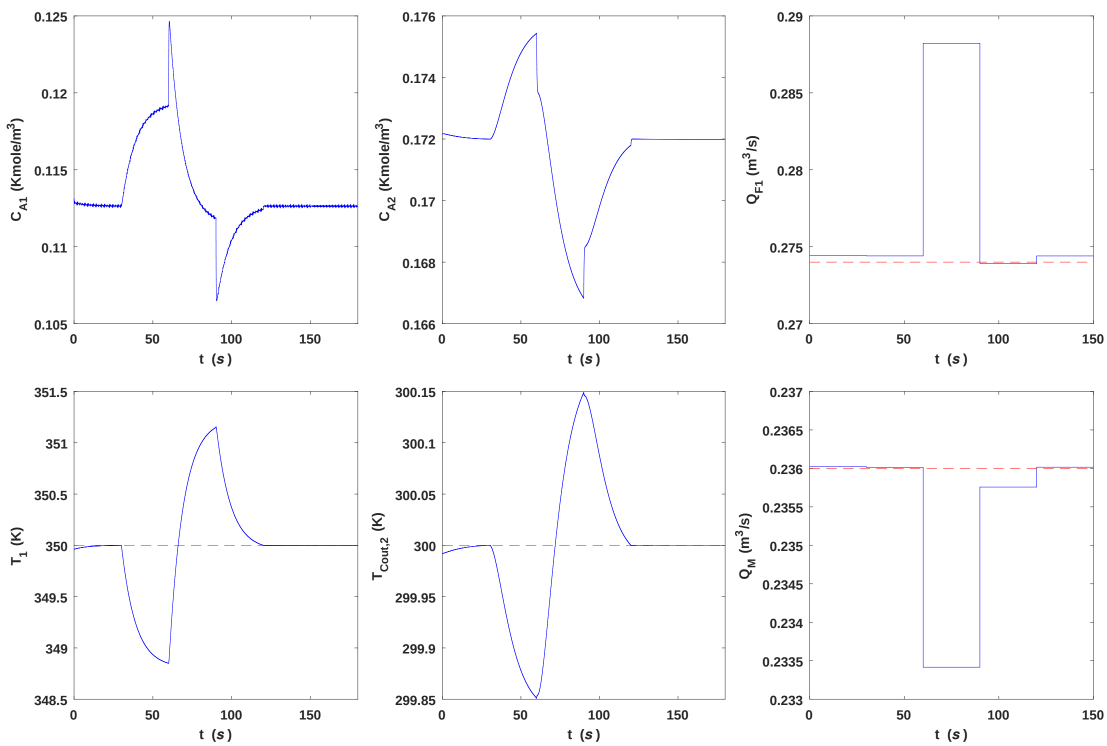

Figure 4.7: Dynamic behavior of the in-series CSTRs for the EMPC optimal process operation ($T_e = 30s$ & $+25\%$ short-term pulse disturbance in $Q_{c,1}$). The output and input variables (——) and the output constraints and optimal steady-state inputs (- - -).

Due to the multilevel optimization problem structure of the economic layer, the number of the economic layer iterations and the size of the optimization problem does not remain the same as that of the open-loop formulation. These values are reported in table (4.6) for the primary economic optimization problem and the MPC subproblems in the CL-DRTO optimization layer. Because of the sequential structure of the CL-DRTO formulation, the total number of the MPC subproblem solution depends on the number of function evaluation of the optimization solver (N_{FE}) for the primary optimization problem. The N_{FE} is not exactly known before solving CL-DRTO in each update time. However, a reasonable number of the N_{FE} less than the default maximum function evaluation could provide an estimate of the expected order of the increase in the solution time. It should pointed that the MPC

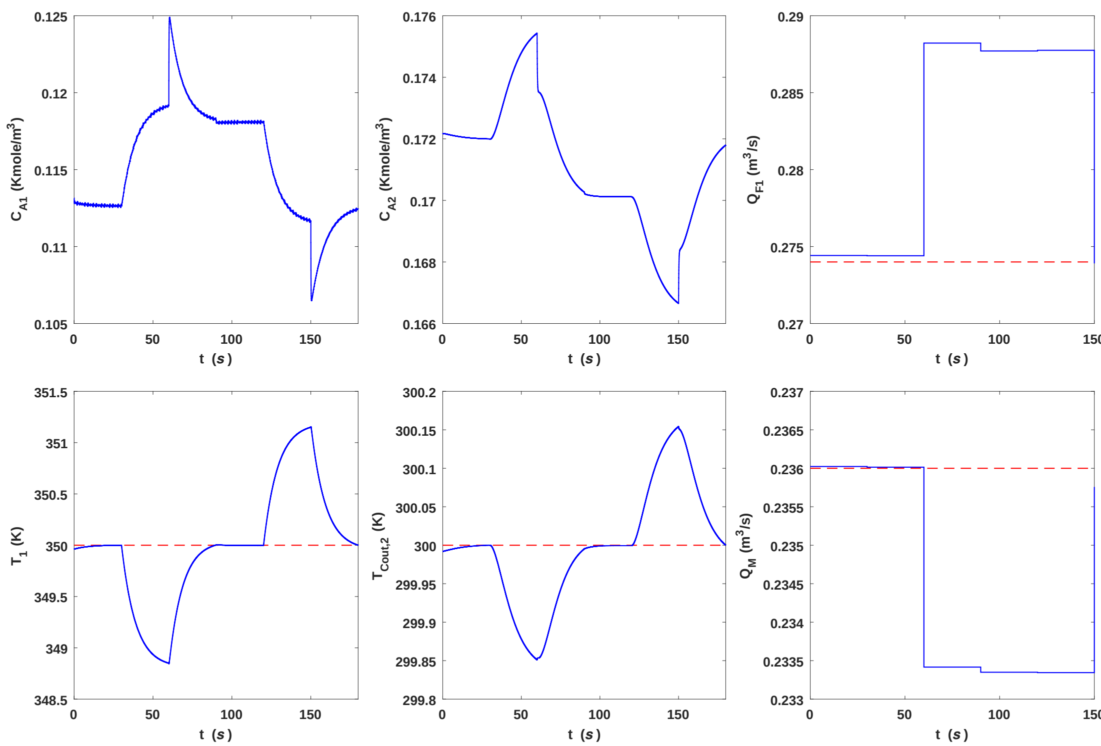

Figure 4.8: Dynamic behavior of the in-series CSTRs for the EMPC optimal process operation ($T_e = 5s$ & +25% sustained pulse disturbance in $Q_{c,1}$). The output and input variables (——) and the output constraints and optimal steady-state inputs (- - -).

subproblems in each CL-DRTO iteration step of the economic optimization layer, are solved to cover the entire economic optimization horizon. As the MPC update time $T_c = 5s$ and the economic optimization horizon $h_e = 60s$, 12 consecutive MPC subproblems fit into the economic optimization time interval. Thus, the number of required MPC subproblem solution in each primary optimization problem of the CL-DRTO step is 12 times the number of function evaluations. There are 6 CL-DRTO step for the entire simulation time ($t_f = 180s$). Therefore, the total number of required MPC subproblem solution is the summation of the number of MPC subproblem solutions for all of the CL-DRTO steps.

Figures 4.14-4.17 show the simulation results of the CL-DRTO-MPC formulation for the chosen disturbance scenarios. Trends of the changes and dynamic behavior of the out-

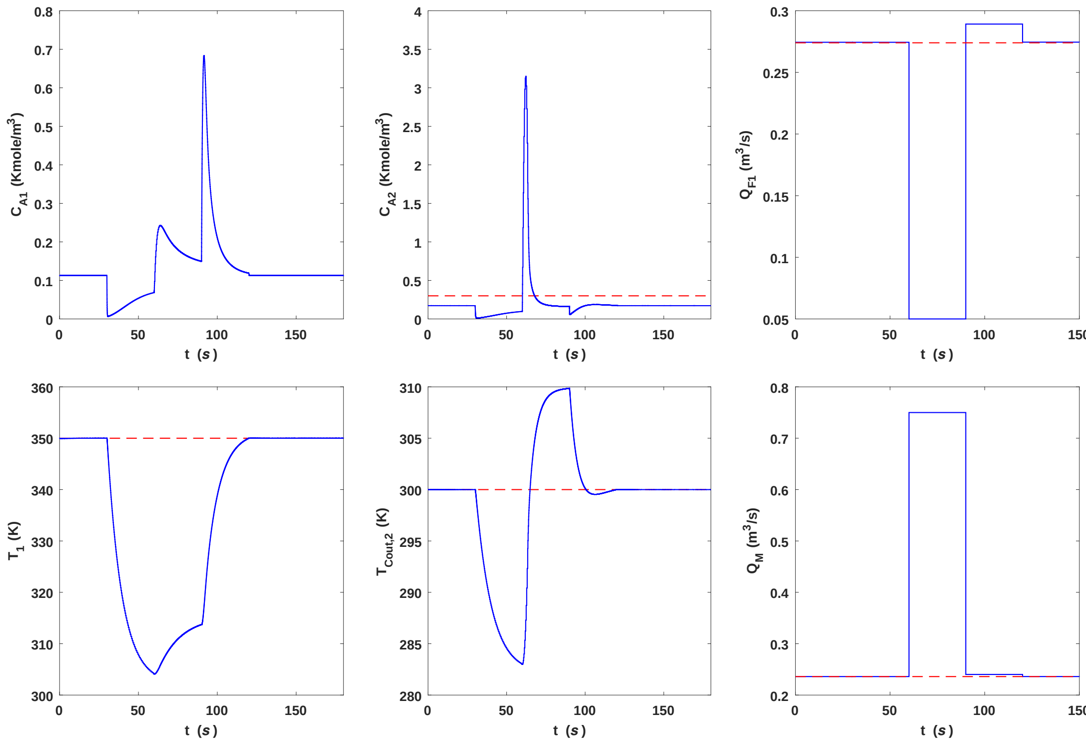

Figure 4.9: Dynamic behavior of the in-series CSTRs for the EMPC optimal process operation ($T_e = 5s$ & -95% short-term pulse disturbance in $C_{A,F1}$ and $C_{A,M}$). The output and input variables (——) and the output constraints and optimal steady-state inputs (- - -).

puts and the performance of the closed-loop formulation are discussed in the performance comparison of the next section.

4.2.4 Performance Comparison

In this section, the resulting economic objective, average run time and cumulative constraint violation of the outputs are reported in tables (4.7, 4.8, 4.9 & 4.10) for the disturbance scenarios. The performance results of the single- and two-layer formulations are discussed for each disturbance scenario separately.

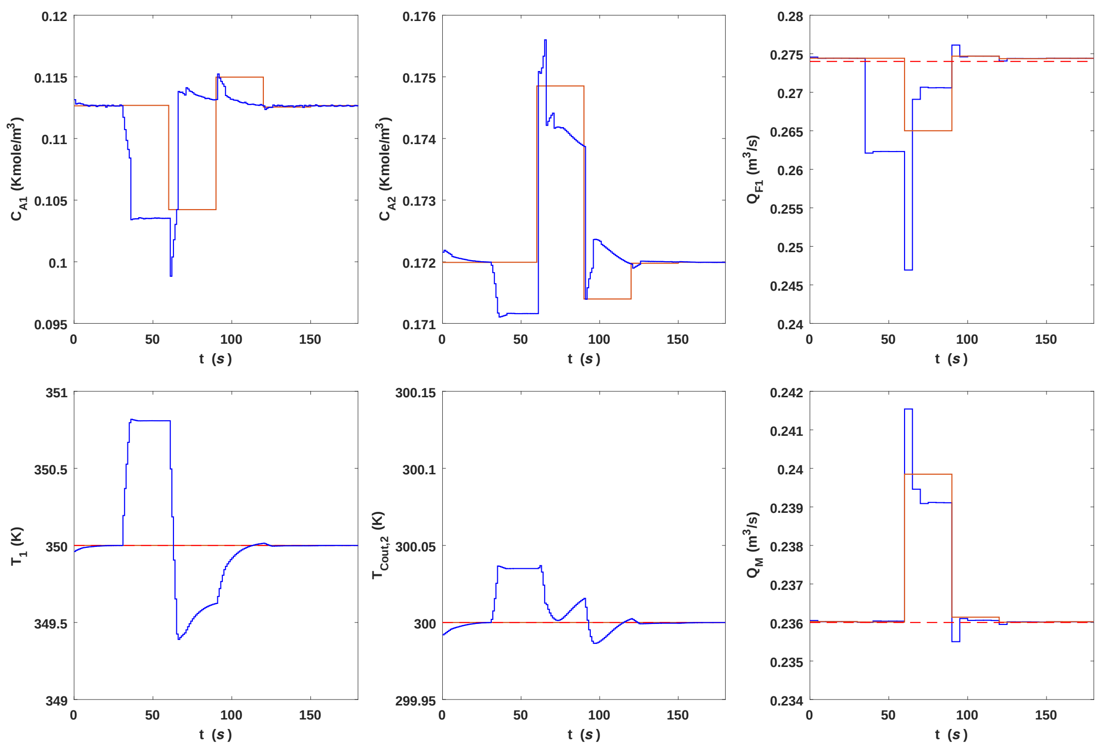

Figure 4.10: Dynamic behavior of the in-series CSTRs for the OL-DRTO-MPC optimal process operation (-25% short-term pulse disturbance in $Q_{c,1}$). The output and input variables (——), optimal input-output reference signals (——), and the output constraints and optimal steady-state inputs (- - -).

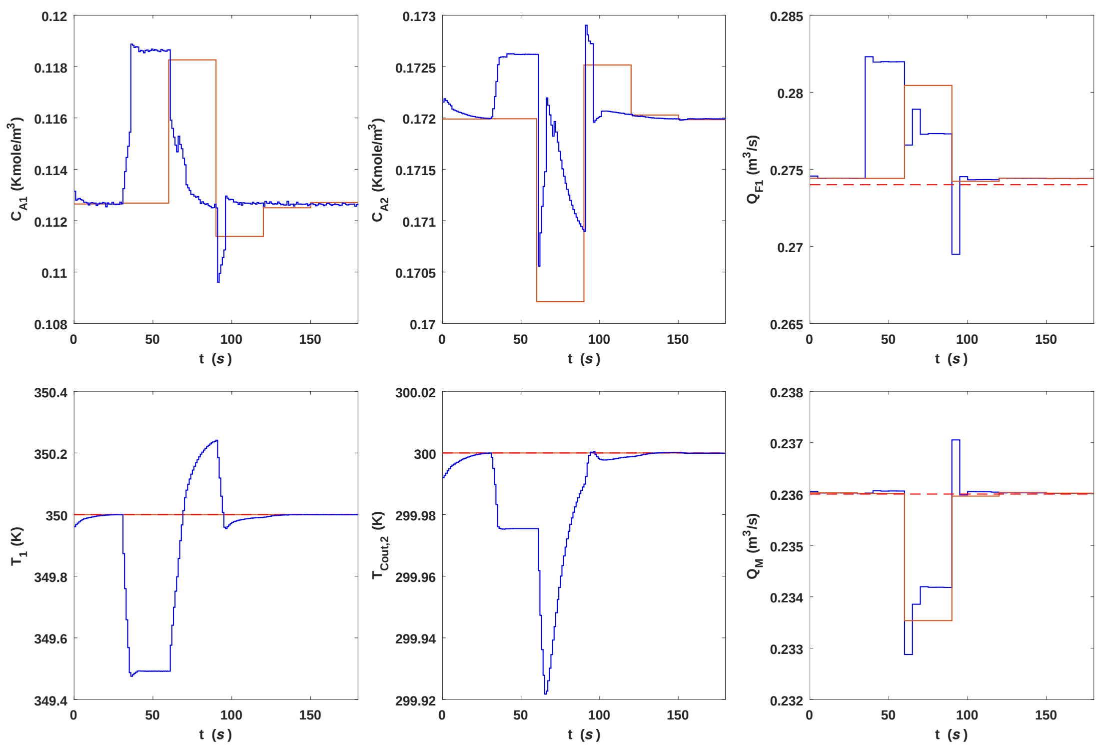

Figure 4.11: Dynamic behavior of the in-series CSTRs for the OL-DRTO-MPC optimal process operation (+25% short-term pulse disturbance in $Q_{c,1}$). The output and input variables (——), optimal input-output reference signals (——), and the output constraints and optimal steady-state inputs (- - -).

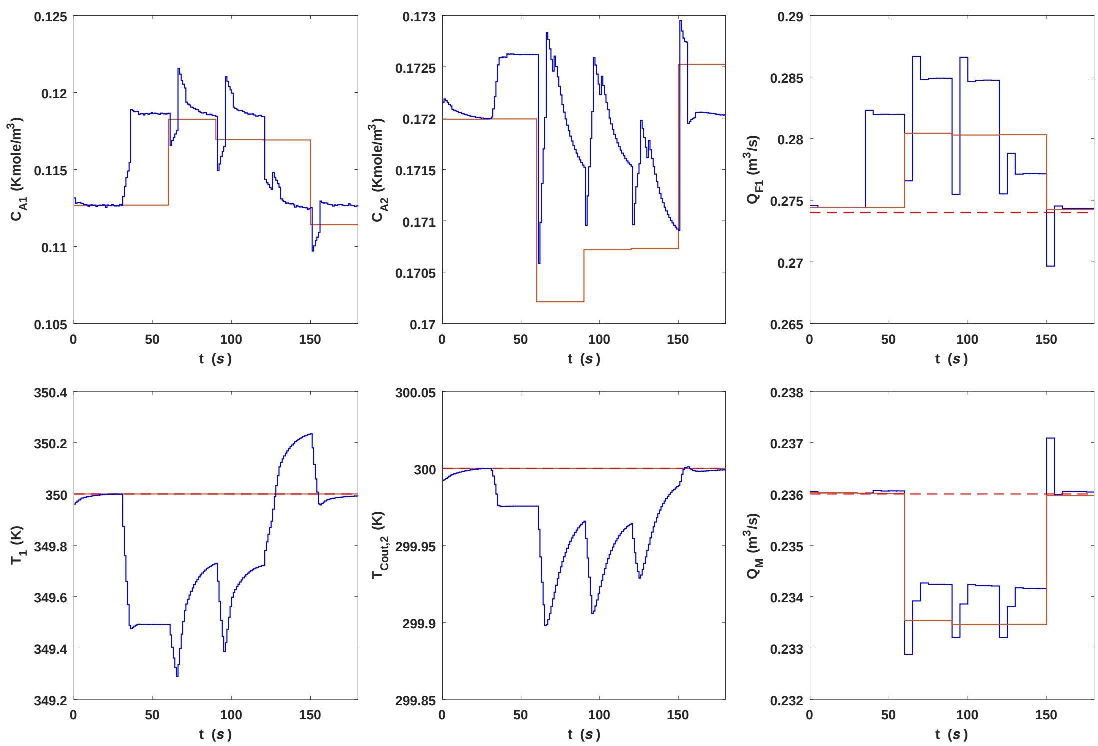

Figure 4.12: Dynamic behavior of the in-series CSTRs for the OL-DRTO-MPC optimal process operation (+25% sustained pulse disturbance in $Q_{c,1}$). The output and input variables (——), optimal input-output reference signals (——), and the output constraints and optimal steady-state inputs (- - -).

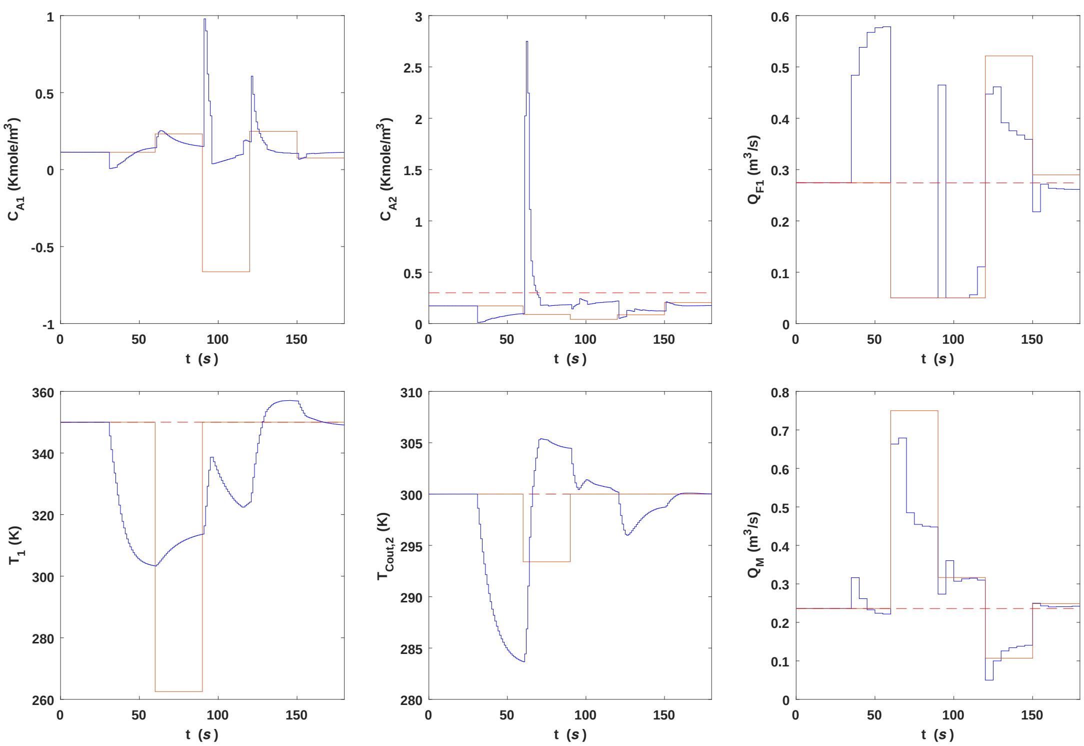

Figure 4.13: Dynamic behavior of the in-series CSTRs for the OL-DRTO-MPC optimal process operation (-95% short-term pulse disturbance in $C_{A,F1}$ and $C_{A,M}$). The output and input variables (——), optimal input-output reference signals (——), and the output constraints and optimal steady-state inputs (- - -).

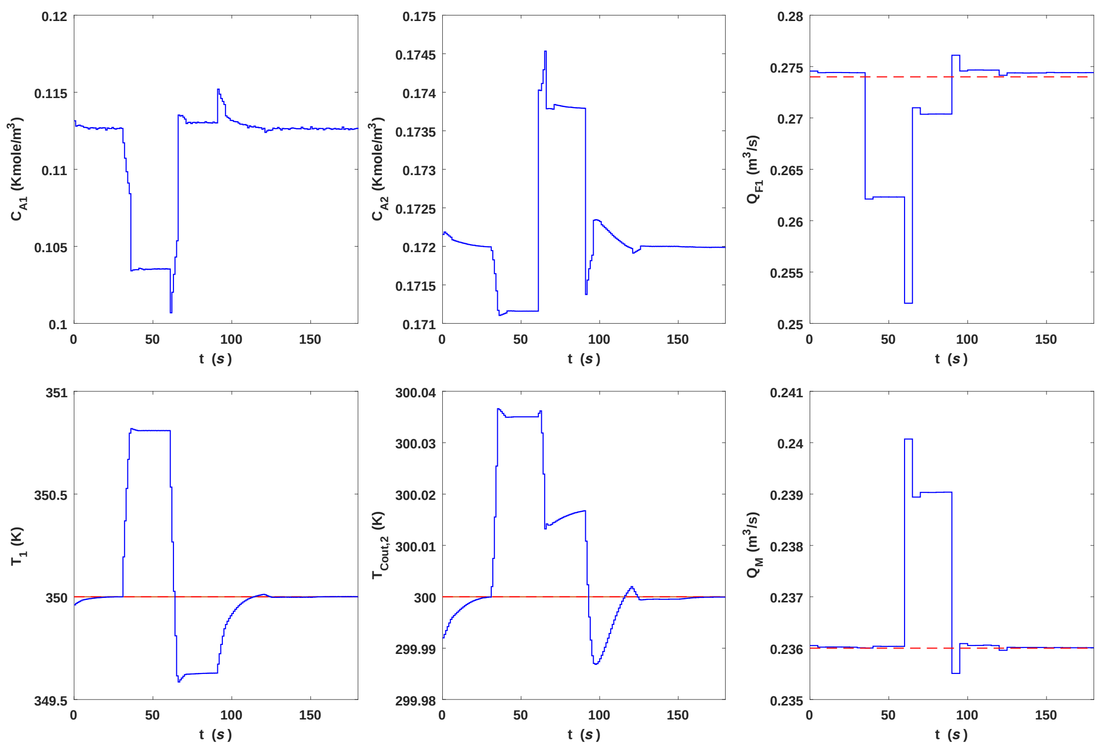

Figure 4.14: Dynamic behavior of the in-series CSTRs for the CL-DRTO-MPC optimal process operation (-25% short-term pulse disturbance in $Q_{c,1}$). The output and input variables (——), optimal input-output reference signals (——), and the output constraints and optimal steady-state inputs (- - -).

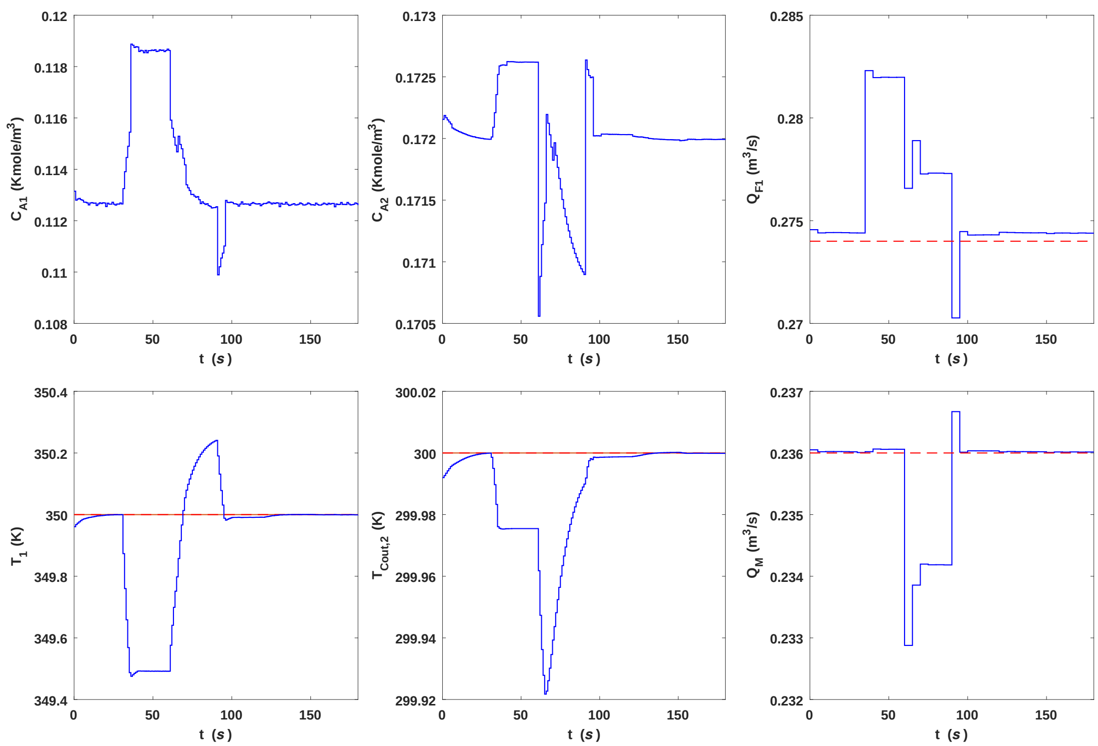

Figure 4.15: Dynamic behavior of the in-series CSTRs for the CL-DRTO-MPC optimal process operation (+25% short-term pulse disturbance in $Q_{c,1}$). The output and input variables (——), optimal input-output reference signals (——), and the output constraints and optimal steady-state inputs (- - -).

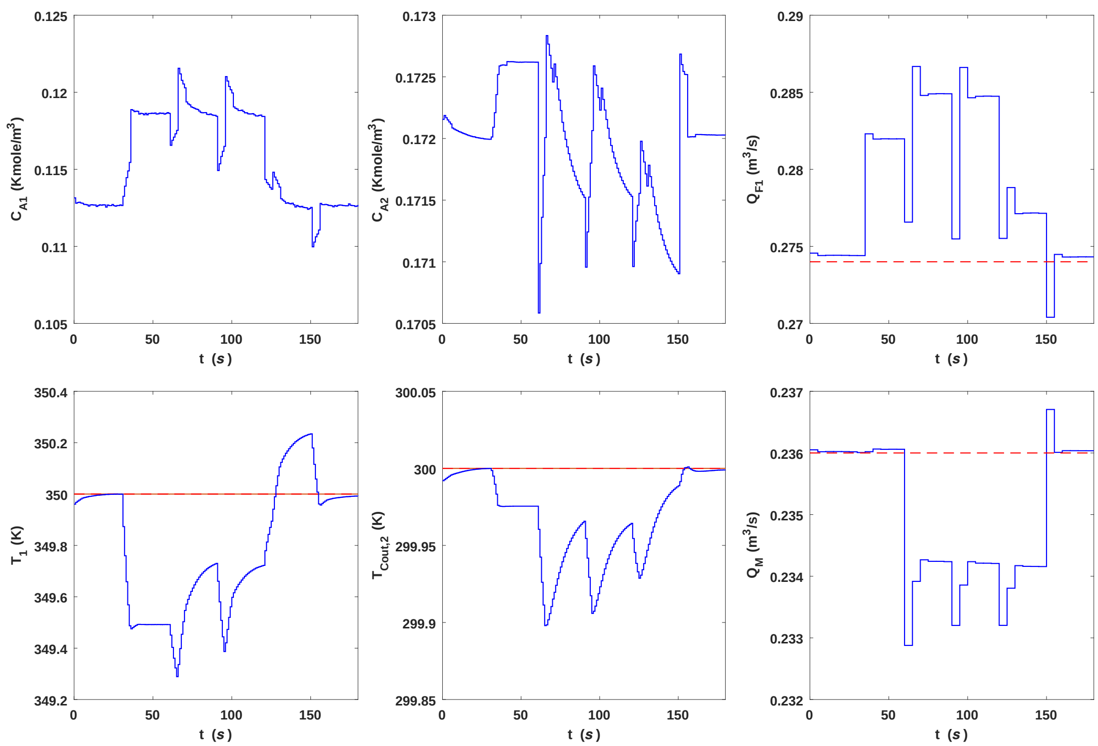

Figure 4.16: Dynamic behavior of the in-series CSTRs for the CL-DRTO-MPC optimal process operation (+25% sustained pulse disturbance in $Q_{c,1}$). The output and input variables (——), optimal input-output reference signals (——), and the output constraints and optimal steady-state inputs (- - -).

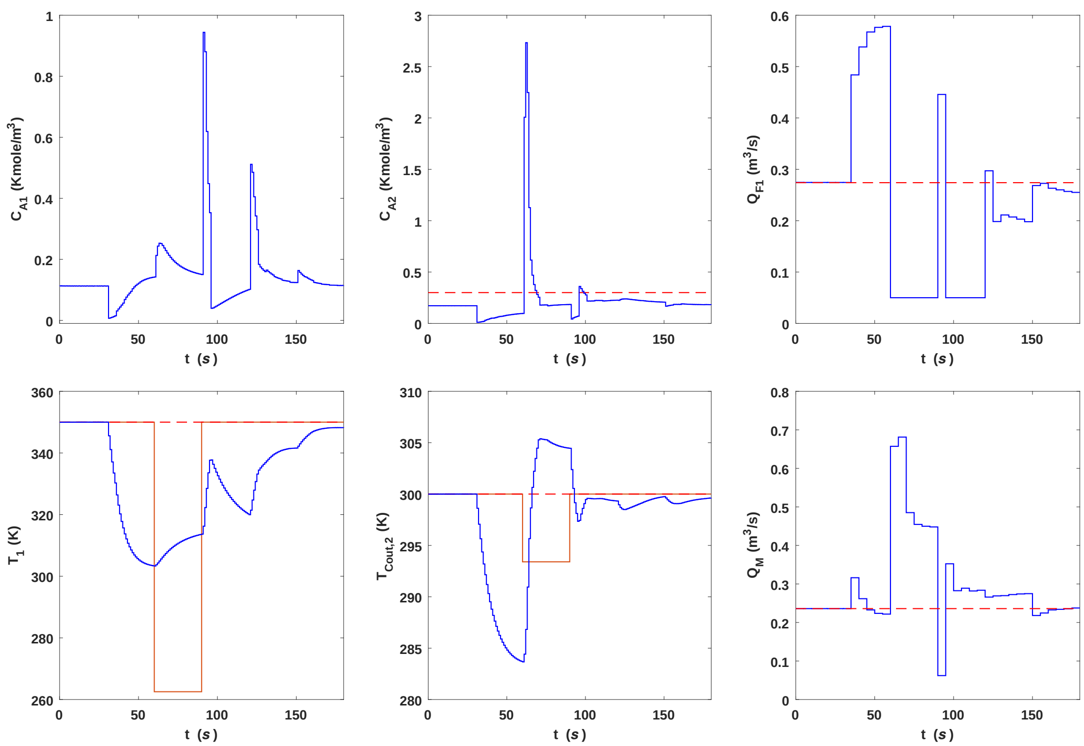

Figure 4.17: Dynamic behavior of the in-series CSTRs for the CL-DRTO-MPC optimal process operation (-95% short-term pulse disturbance in $C_{A,F1}$ and $C_{A,M}$). The output and input variables (——), optimal input-output reference signals (——), and the output constraints and optimal steady-state inputs (- - -).

Table 4.6: CL-DRTO-MPC design parameters and associated NLP-QP subproblems & QP problem sizes and number of their iteration steps for $t_f = 180s$

Automation level		Parameters		Problem sizes & iteration steps	
CL-DRTO	Primary problem	$T_e = 30s$	$N_e = 2$	$N_{NLP} = 4$	$N_{Iter} = 6$
	MPC subproblems	$T_c = 5s$	$N_c = 6$		
		$Q = I_{2\times2}$	$\Gamma = 0_{2\times2}$	$N_{QP} = 12$	$^{\dagger}N_{Iter} = \sum_{i=1}^{6} 12N_{FE}^{i}$
		$S = 0.01I_{2\times2}$			
MPC		$T_c = 5s$	$N_c = 6$		
		$Q = I_{2\times2}$	$\Gamma = 0_{2\times2}$	$N_{QP} = 12$	$N_{Iter} = 36$
		$S = 0.01I_{2\times2}$	$w_c = 10^6$		

† N_{FE}^{i} denotes for the number of function evaluation that is required to solve the primary NLP in ith CL-DRTO iteration step.

Negative short-term disturbance in Q_{c1}

A sudden pulse decrease in the coolant flow rate of the first CSTR reactor reduces the cooling effect and consequently causes an increase in the temperature of the first reactor and the temperature of the coolant outlet stream in the second CSTR reactor. This negative short-term pulse is used to simulate an undesired condition in which an unknown disturbance causes the output signals to escape the admissible operating region. Therefore, it is expected to observe a feedback regulation function in the EMPC similar to that of the MPC layer in the two-layer methods (Bartusiak [2007]) to counter this undesired effect of the disturbance. Moreover, an increase in the CSTR and/ or coolant outlet temperature indicates a higher rate of the exothermic reactions. Also, an increase in the reactant concentration in the reactors could increase the rate of the desired reaction and consequently improve the economic performance in this case study. However, the increase of these output variables in the current disturbance scenario leads to a significant safety and operation constraint violations for the two-layer methods and the EMPC with the slower update frequency. Thus, the higher constraint violation causes a higher economic performance in this scenario. In this case, it is only intended to show the constraint violation effect for the economic optimization problem with the larger update time in the presence of an unknown disturbance scenario. Hence, the economic performance comparison is not considered for this disturbance scenario. Figures 4.2, 4.6, 4.10 and 4.14 show different regulation functions in terms of the maximum violation of the safety and operating temperature constraint in the CSTRs. In figure 4.2, the EMPC with the smaller update time ($T_e = 5s$) reacts to the utility resource limitation of the first CSTR by decreasing the inlet feed flow rate (Q_{F1}) and increasing the second manipulated variable (Q_M). Safety constraint and operation constraint violations are observed in T_1 and T_{c2out} subplots due to the unknown disturbance effect. Similar patterns for the manipulated inputs and output temperature changes are observable in figure 4.6. However, the maximum output constraint violation and COCVs for the larger economic update time $T_e = 30s$ are larger than those of the EMPC with the smaller update time. The first manipulated input (Q_{F1}) in the results of the open- and closed-loop dual layer methods in figures 4.10 and 4.14 gradually changes to decrease the constraint violations. A lower maximum constraint violation is also observed for the dual-layer method comparing to that of the EMPC with the larger update time. Table (4.7) shows the quantitative metric for each constraint violation of the single- and two-layer formulations. The qualitative regulation performance comparison from the graphs and the tabulated results show that an EMPC formulation with a larger update time could cause a severe constraint violation. This issue was predicted by Ochoa *et al.* [2010] for the larger updating time gap in the single-layer method which was referred to as the dead period. Thus, this results signify the necessity of the MPC control layer for the larger economic update time.

Amrit *et al.* [2013] showed that the regulation performance of the EMPC and MPC controller are different. This is due to the facts that regulatory and economic operation mechanisms of EMPC and MPC use different objective functions and may act on the system in opposite directions. Therefore, the EMPC automatically compromises between the required regulatory efforts and economic optimal operation to maintain the system within the admissible operating region and leads to an improved economic performance.

Table 4.7: Performance comparison in the presence of 25% short-term negative pulse disturbance in $Q_{c,1}$.

Method	$\Phi_{eco}(£)$	$ART(s)$	$COCV_{T_1}(Ks)$	$COCV_{T_{c2out}}(Ks)$
EMPC ($T_e = 5$)	15507.91	380.19	3.99	0.19
EMPC ($T_e = 10$)	15507.53	36.90	12.84	0.99
EMPC ($T_e = 20$)	15527.70	7.19	34.11	3.88
EMPC ($T_e = 30$)	-*	2.18	55.75	7.19
OL-DRTO-MPC	15519.27	3.85	24.31	1.53
CL-DRTO-MPC	15522.18	7.37	24.29	1.53

Jamaludin and Swartz [2015] show that the CL-DRTO-MPC responds to the change faster than the OL-DRTO-MPC. This feature could improve the economic performance. Jamaludin and Swartz [2016] also show that CL-DRTO could provide a constraint back-off mechanism to avoid constraint violation. However, the constraint violation results of the CL-DRTO in table 4.7 do not show any improvement over that of the OL-DRTO-MPC method. This indicates that the MPC controller-process model interaction does not have a significant effect on the output prediction. Figure 4.19 shows that the open-loop and closed-loop temperature output prediction for the current disturbance scenario are slightly different. However, this difference is negligible comparing to the different output prediction results in the presence of the third disturbance scenario (figure 4.20). The quantitative results of table 4.11 confirms that the prediction errors for the $Q_{c,1}$ disturbance scenarios have the same order of magnitude, whereas the prediction error for the disturbance in feed concentration has higher order of magnitude in comparison to the $Q_{c,1}$ disturbance scenarios. Thus, the effect of embedding closed-loop model in the DRTO layer is only observed for the disturbance in the feed concentration and the performance of the CL-DRTO-MPC does not considerably change in comparison to that of the OL-DRTO-MPC formulation in the presence of the $Q_{c,1}$ disturbance scenarios. This effect would be explained in more details in the next section.

The average CPU run times for a time interval which is equal to $T_e = 30s$ are reported in table 4.7 for each method. The ART for the EMPC method with the smaller update time is two orders of magnitude higher than that of the other methods. The ART of the EMPC shows that considering the update time $T_e = 5$ and the highest average solution for the EMPC updates, the real-time application of the single-layer EMPC method using the existing formulation may cause difficulty. Also a large computational delay could reduce the economic performance and stability of the process (Yang and Biegler [2013]). However, the advanced-step and advanced-multi-step methods could mitigate the computational delay effects especially when slowing down the sampling rate is a less suitable option, as it will degrade the performance of the EMPC (Zavala and Biegler [2009a] and Yang and Biegler [2013]).

There is a possibility to reduce the dynamic optimization problem size by increasing the economic optimization update time. Accordingly, the resulting NLP problem solution time could be reasonably reduced for the real-time application. This possibility leads to the case study problems for the EMPC implementation with intermediate update times $T_e = 10$ and $20s$. The ART results in table 4.7 shows the reduction in the solution time. However, comparing the COCV results of table 4.7 for the EMPC formulations with different update time verifies that the constraint violation could increase as a result of the increase in the economic update time. The higher COCV results confirm the prediction of Ochoa *et al.* [2010] that the single-layer method with a larger update gaps could be more susceptible to the constraint violation effects of the unknown disturbances.

It is assumed that the economic performance for an average safety temperature constraint violation higher than 0.2 and an average product quality constraint violation higher than 0.01 are not acceptable. For the current disturbance scenario in table 4.7, the COCV results of the EMPC with the update times $T_e = 20$, and $30s$ are higher than those of the two-layer methods. Also, the higher COCV of the EMPC with $T_e = 30s$ could breach the tolerable constraint violation limits and consequently cause unacceptable economic performance.

The ARTs for the two-layer methods and the EMPC with larger update time have the same order of magnitude. The optimization problem sizes and number of required NLP and QP optimization problem in a certain time interval of $T_e = 30s$ explain why the magnitude of the ART in one method is higher than that of the others. The effects of these factors are mentioned in the previous section for each formulation. The ART for the EMPC with larger update time which is lower than the ART for the OL- and CL-DRTO-MPC formulation is consistent with the expected effects. For example, in the OL-DRTO-MPC formulation several QP problem must be solved in addition to the NLP problem, while there is no QP problem in the EMPC method. Also, in the closed-loop formulation the solution time of the QP subproblems in the multi-level optimization problem of the CL-DRTO layer contributes to the higher ART result in comparison to that of the open-loop formulation.

Positive short-term disturbance in Q_{c1}

In the simulation results of figures 4.3, 4.7, 4.11 and 4.15 a sudden pulse increase in the coolant flow rate of the first CSTR reactor causes a temporary over-cooling effect. The over-cooling effect causes a temperature drop in the first reactor and the coolant outlet stream in the second CSTR reactor. As a result the pulse increase in the utility resource flow rate provides an extra raw material processing capacity. This extra processing capacity could be exploited by increasing the reactor temperatures in the allowable temperature range. Therefore, there is an opportunity for the use of the real-time optimization methods to increase the net profit. The economic performance results of table 4.8 shows that the EMPC method with the smallest update time achieves slightly higher profit in comparison to the two-layer methods. The economic performance superiority of the EMPC is because of the smaller economic update time in the feedback structure which results a prompt adjustment of the input feed flow rate to increase the profit. This result confirms the economic performance comparison findings in the work of Ochoa *et al.* [2010] which states that the single-layer formulation reacts to the changes of the unknown disturbance faster than the two-layer formulation. However, the difference between the performance improvement of the single-layer and two-layer formulation is negligible. Therefore, a faster update time is not necessary for the economic performance improvement. The open- and closed-loop two-layer formulations lead to an equal economic performance. This equal economic performance represents a situation similar to the previous scenario in which, the CL-DRTO-MPC may not enhance the economic performance comparing to the OL-DRTO-MPC in the presence of the unknown disturbance. The effect of unknown disturbance is explained for the COCV result comparison of the open- and closed-loop formulations in the next paragraph.

Table 4.8: Performance comparison in the presence of 25% short-term positive pulse disturbance in $Q_{c,1}$.

Method	$\Phi_{eco}(£)$	$ART(s)$	$COCV_{T_1}(Ks)$	$COCV_{T_{c2out}}(Ks)$
EMPC ($T_e = 5$)	15620.35	321.22	2.59	0.13
EMPC ($T_e = 10$)	15619.98	41.16	8.13	0.66
EMPC ($T_e = 20$)	15603.27	5.91	21.33	2.44
EMPC ($T_e = 30$)	15619.03	2.75	34.51	4.47
OL-DRTO-MPC	15599.96	2.88	4.31	0.00
CL-DRTO-MPC	15600.12	8.88	4.31	0.00

The simulation results of figure 4.3, shows the limited time T_1 safety constraint violation for the EMPC with the smaller update time, while a more sustained constraint violation is observed for T_1 in figure 4.7 as a result of larger economic update time. Also the maximum T_1 constraint violation is higher than that of the EMPC with the smaller update time. A similar constraint violation pattern is observed for T_{c2out} in figures 4.3 and 4.7. T_1 constraint violation results for dual-layer formulations in figures 4.11 and 4.15 are less than that of the EMPC with the larger update time. Also, the manipulated input Q_{F1} in the results of dual-layer formulations in figures 4.11 and 4.15 reacts earlier than that of the EMPC with the larger update time.

The EMPC feedback structure requires at least one economic update time to capture the unknown disturbance effect using the feedback approach for the model parameter updates. The EMPC with the larger update time shows a sluggish regulation function due to the bigger feedback update delay. As a result of the larger update time a severe constraint violation occurs for the output temperatures in the EMPC formulation with $T_e = 30ss$ (see table 4.8 for COCV results). Comparing to the EMPC with a large update time, the MPC controller in the two-layer formulations could reduce the undesired constraint violation. However, in the two-layer methods the COCV is slightly higher than that of the EMPC with smallest update time. These slightly different COCVs could be the result of the fact that the MPC control layer in the dual-layer methods uses a linearized model of the process. While, the EMPC with an update time equal to that of the MPC control layer uses a nonlinear model of the process.

The CL-DRTO-MPC formulation could recognize the future model mismatch between the nonlinear model of the economic layer and linear MPC predictions and correct it using the MPC model bias update based on the nonlinear model. Therefore, closed-loop formulation could adjust the setpoint trajectories in such a way that the closed-loop predictions will return the best economics (Jamaludin and Swartz [2016]). A detailed investigation of the OL- and CL-DRTO MPC performances in the next section would reveal that there is no considerable difference between the open- and closed-loop model prediction in the presence of the current disturbance scenario. Thus, the closed-loop variant of the two-layer method, which could moderate constraint violation with a DRTO-MPC model discrepancy root cause, does not have any advantages over the OL-DRTO-MPC formulation (see table4.8). In this case, the unknown nature of disturbance might be the only dominant reason for the constraint violation for both of the dual-layer methods.

The average CPU run times for a time interval which is equal to $T_e = 30s$ are reported in table 4.8 for each method. The trend of change in the ART results from one method to the other methods is similar to the ART for the previous unknown disturbance scenario. Likewise the ART results of the previous section for the EMPC with the smallest update time, the large computational delay may impair the economic performance and the regulatory function in the process operation. The observation of ART results for the larger T_e shows the reduction in the computational load comes at a cost of higher constraint violations. It is pointed that the EMPC with the largest update time $T_e = 30$ results the highest constraint violation. Also, the increase in the update time leads to a slightly lower profit in the cases that the COCV is in the reasonable range.

The ARTs for the dual-layer methods and the EMPC with the larger update times ($T_e = 20$ and $30s$) have the same order of magnitude. The same reasoning stands for the explanation of the difference in the order of magnitude of the ART in the single- and dual-layer formulations.

Positive sustained disturbance in Q_{c1}

The unknown sustained pulse increase in the utility flow rate provides an extra raw material processing capacity for the same reason that is discussed in the previous comparison for the short-term disturbance scenario. The unknown sustained increase in the coolant flow rate of the first reactor means that the extra coolant utility resource is available over the longer period of the process operation time comparing to the improvement capacity of the short-term version of the disturbance. Therefore, for the sustained disturbance scenario, it is expected to achieve a higher economic performance improvement in comparison to the previous disturbance scenario due to the longer duration of the unknown pulse disturbance. A comparison between the values of Φ_{eco} for each method in tables 4.8 and 4.9 shows different effects of the sustained and short-term disturbance changes on the economic performances. Despite the difference between the economic performance of each method in the presence of the short-term and sustained disturbances, table 4.9 shows that the order of the higher to lower economic performance is similar to that of the previous disturbance scenario. The economic performance of the EMPC with the smallest update time is slightly higher than that of the CL-DRTO-MPC and OL-DRTO-MPC. The economic performance results of table 4.9 shows that the economic performance deterioration due to the increase in the economic update time is negligible in the EMPC methods. However a smaller COCV could be achieved because of the smaller economic update time. This results are consistent with the comparison results of the previous disturbance scenario.

Table 4.9: Performance comparison in the presence of 25% sustained positive pulse disturbance in $Q_{c,1}$.

Method	$\Phi_{eco}(£)$	$ART(s)$	$COCV_{T_1}(Ks)$	$COCV_{T_{c2out}}(Ks)$
EMPC ($T_e = 5$)	15708.77	273.67	2.59	0.13
EMPC ($T_e = 10$)	15708.42	38.04	8.13	0.66
EMPC ($T_e = 20$)	15691.52	9.22	21.44	2.54
EMPC ($T_e = 30$)	15707.33	2.21	34.61	4.63
OL-DRTO-MPC	15652.00	2.71	4.67	0.00
CL-DRTO-MPC	15652.14	8.75	4.68	0.00

The COCV results of table 4.9 are similar to the constraint violation of the short-term disturbance scenario. The same interpretations is still valid in the reasoning of the different constraint violations criteria. The difference in the COCV of the OL- and CL-DRTO is discussed in the next section.

Also, a similar ART pattern can be seen for the sustained disturbance scenario for the application of the single- and dual-layer methods. However, the average CPU time for the sustained disturbance is slightly less than that of the short-term disturbance scenario for each method. This results are also obtained by Amrit *et al.* [2013] for the lower frequency of unknown disturbance changes. The lower ART results are obtained because of a warm start initialization of the interior-point method. The warm start initialization is constructed from the solution of the previous NLP problems.

Negative short-term disturbance in $C_{A,F1}$ and $C_{A,M}$

Since the inlet feed stream is shared by the two CSTRs in this case study problem, a disturbance change appears in both of the inlet feed concentrations. A sudden decrease in the feed concentration leads to a lower reactant concentration in the reactors. The lower concentration of the reactants decreases the conversion rate of A in equations 4.2 for both of the reactors. The lower exothermic reaction rates produce less heat. As a result, considering the effect of reaction rates in the heat balance equations 4.3, reactor temperatures should drop which is similar to the effect of the increase in the utility flow rate of the first reactor. The reduced temperature effect in turn decreases the rate of the conversion of the reactant A. According to the Arrhenius type temperature dependency $k_j(T_i) = k_{0,j}exp(-\frac{E_j}{RT_i})$, rate of the desired reaction $A \longrightarrow B$ decreases faster than that of the undesired reaction $B \longrightarrow C$ because of the higher activation energy (see table 4.1). Therefore, an increase in the volumetric feed flow rate, which is the manipulated variable, could accelerate the exothermic reaction to oppose the temperature drop in the reactors. However, this change in the feed concentration may not necessarily increase the total raw material (i.e. total molar feed flow of A) processing capacity. Figure 4.5 shows the changes in the manipulated inputs Q_{F1} and Q_M in response to the disturbance for the EMPC with the smaller update time. In response to the unknown disturbance effects, the lower bound constraint for the first input (Q_{F1}) and the total feed flow rate constraint of equation 4.12 are active constraints for a certain simulation time interval. In this case study problem, the online economic optimizer decides to decrease the volumetric inlet feed flow rate of the first CSTR to its minimum value and injects the feed with the highest available flow rate directly into the second CSTR. The EMPC controller uses the saturated input changes to resist the rapid decrease in the output temperature T_1 and T_{c2out}. The general trend of the input responses could be explained as an optimal allocation of the available flow rate between the two possible feed inlet positions to avoid over-cooling of the raw material in the first reactor before feeding it to the second CSTR. The over-cooling could have a negative effect on the production rate of the desired product B in the second CSTR and the cooling utility cost of the first CSTR. However, it may not be easy to intuitively predict the behavior of each individual input response. Also, a quality constraint violation is observed for the reactant concentration in the second reactor $C_{A,2}$ which is regulated using the manipulated inputs Q_{F1} and Q_M. There is a similar interpretation of the input changes in figure 4.9 for the EMPC with the larger update time. However, the manipulated input actions are delayed comparing to the Q_{F1} and Q_M input changes in figure 4.5. As a result, the EMPC with the larger update time shows a sluggish regulation function due to the delayed input responses. This sluggish regulation function causes a large output temperature (T_{c2out}) constraint violation for the EMPC with the larger update time (see figure 4.9). The simulation results of the open- and closed-loop DRTO formulations in figures 4.13 and 4.17 show a slightly different input change strategy for the first input action (Q_{F1}). In these figures Q_{F1} is initially increased before decreasing to the minimum inlet feed flow rate. The maximum constraint violation for the output temperature T_{c2out} in figure 4.13 is smaller than that of the EMPC with the larger update time in figure 4.9. Also, the COCV of the T_{c2out} output in the closed-loop formulation results of figure 4.17 is smaller than that of the open-loop formulation results in figure 4.13.

The economic performance results of table 4.10 show that the EMPC method with a smallest update time has a higher profit comparing to that of the closed-loop two-layer formulation. Table 4.10 also shows that the economic performance of the EMPC methods with the larger update times and the open-loop two-layer formulation are not credible because the constraint violation of the product specification and safety temperature of the first reactor are significantly higher than the tolerable limits, which are mentioned in the result comparison of the negative short-term disturbance scenario.

The COCV results of the EMPC formulation increase with the increase in the update time due to the same reason which is interpreted for the previous disturbance scenarios. The MPC control layer in the OL-DRTO-MPC method could successfully reduce the $C_{A,2}$ quality constraint violation in comparison to the EMPC with the larger update times. However, the MPC regulation of the OL-DRTO-MPC method causes an inevitable safety temperature constraint violation in the first CSTR reactor. Also, there is a discrepancy between the COCV results of the dual-layer methods and the EMPC with the smaller update time

Table 4.10: Performance comparison in the presence of 95% short-term negative pulse disturbance in $C_{A,F1}$ and $C_{A,M}$

Method	$\Phi_{eco}(£)$	$ART(s)$	$COCV_{T_1}(Ks)$	$COCV_{T_{c2out}}(Ks)$	$COCV_{C_{A,2}}(kmols/m^3)$
EMPC ($T_e = 5$)	13824.44	463.15	0.00	3.08	1.13
EMPC ($T_e = 10$)	-*	41.73	0.00	67.80	6.64
EMPC ($T_e = 20$)	-*	6.84	0.00	190.64	6.70
EMPC ($T_e = 30$)	-*	2.23	0.00	295.45	8.19
OL-DRTO-MPC	-*	10.18	168.76	145.56	1.55
CL-DRTO-MPC	13054.45	19.77	0.00	132.62	1.33

($T_e = 5s$). Since the MPC controller in the 2-layer formulation has the same update time as the EMPC method a similar COCV results are expected. It should be recognized that the MPC controller in the 2-layer formulation uses a linear process model to perform the regulation task whereas the EMPC formulation uses a nonlinear model of the process. It is clear that the closed-loop formulation could mitigate discrepancy between the dynamic models in the DRTO and MPC layers. A detailed observation of the T_{c2out} constraint violation in figure 4.17 which occurs at $t = 70s$ shows that the Q_M input to T_{c2out} output process gain might be underestimated in the linear model of the MPC. As a result of the underestimated gain, the MPC controller introduces a Q_M flow rate which is higher than the required input action and consequently leads to the higher COCV, while the nonlinear model in the EMPC with the smaller update time could provide a higher accuracy of the output prediction. The Q_M input to T_{c2out} output process gains for the nonlinear and linear model are $\kappa_{Nonlinear} = 50.66(Ks/m^3)$ and $\kappa_{Linear} = 37.78(Ks/m^3)$. The input-output gain for the linear model is smaller than that of the nonlinear model. This comparison confirms that the use of linear model in the MPC controller of the 2-layer formulation causes a larger COCV for the closed-loop dual layer method in comparison to that of the EMPC formulation.

Despite the fact that the economic performance of of the EMPC formulation with larger update times and the open-loop two-layer method are not acceptable because of the severe constraint violation, including the COCV results of these methods in table 4.10 is beneficial to illustrate different mechanisms of the constraint violation and the advantage of the closed-loop DRTO method over the open-loop DRTO and single-layer methods with different update times. Unlike the COCV comparison results of the OL- and CL-DRTO-MPC formulations for the previous disturbance scenarios, the closed-loop formulation of the two-layer method results lower COCVs for the coolant temperature of the second reactor and the product quality constraint in comparison to the open-loop formulation. Also, the closed-loop formulation eliminates the COCV of the safety temperature constraint. The elimination of COCV for T_1 shows that the constraint violation arises from the huge difference in the open-loop and closed-loop model prediction of the DRTO layer due to the interaction effects of the embedded MPC controllers and the process model. This difference in the open-loop and closed-loop model prediction of the economic optimization layer is investigated in the next section.

The ART results of table 4.10 shows that the ART of the EMPC for the smallest economic update time is one order of magnitude higher than that of the CL-DRTO-MPC method in the presence of current disturbance scenario. Despite the fact that the EMPC could react faster to the large disturbance to improve the profit and maintain the process within the admissible operating region, the high ART could cause difficulty due to the delay in real-time implementation of the optimal inputs (Yang and Biegler [2013]). However, the advanced-step and advanced-multi-step methods could mitigate the computational delay effects especially when slowing down the sampling rate is a less suitable option, as it will deteriorate the performance of the EMPC (Zavala and Biegler [2009a] and Yang and Biegler [2013]).

4.2.5 Effect of the Open- and Closed-loop Prediction on the Performance of the Dual-layer Methods

The open-loop model of the process in the economic optimization layer cannot capture the closed-loop interaction effects of the MPC control layer and the process model. These interaction effects of the controller and process model are formed because of the controller attempts to regulate the outputs to the setpoints. Depending on the disturbance magnitude and the disturbance input to the temperature and concentration output relative gain, these interactions could lead to a different output prediction. The open-loop and closed-loop process model prediction strategies of figure 4.18, which are used in the real-time economic optimization layer, are compared in this section. The comparison is carried out for a fixed input-output set-point and different disturbance scenarios which are used in the performance comparison of the single- and dual-layer methods.

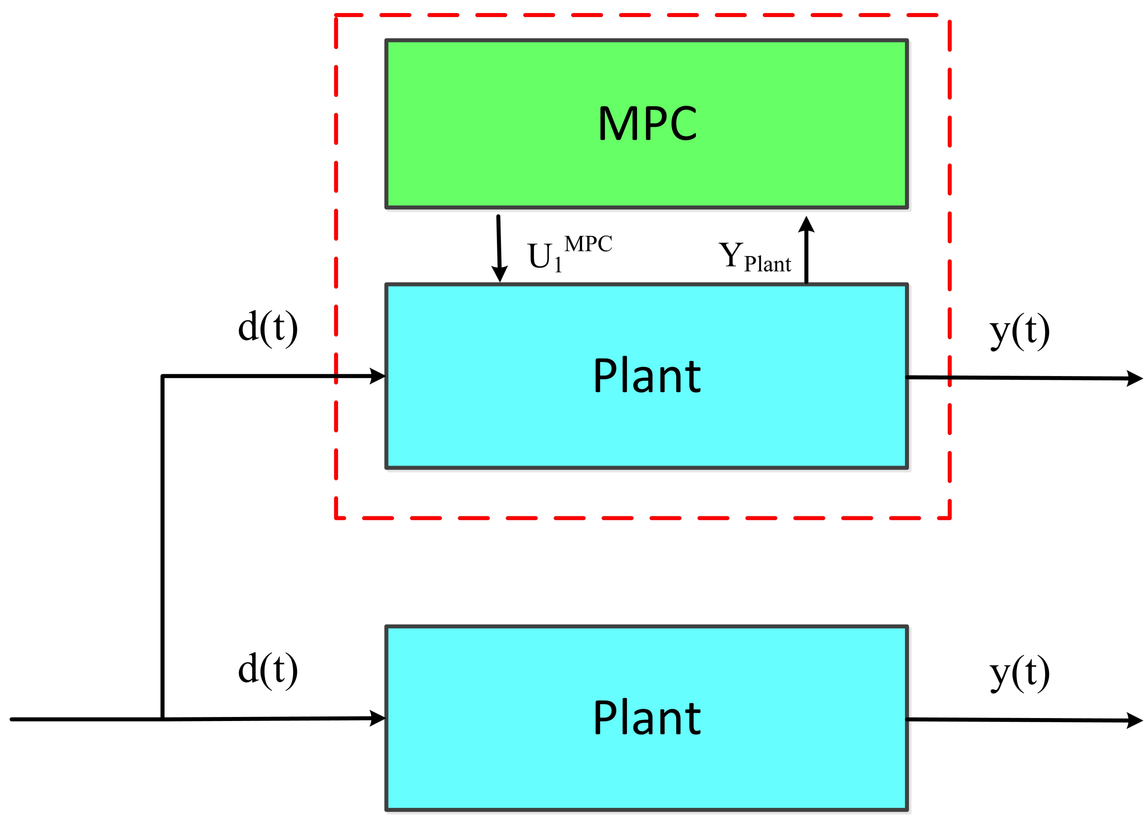

Figure 4.18: Open-loop and closed-loop prediction models of the economic optimization.

The open- and closed-loop prediction differences are quantified and reported in the form of cumulative error in the predicted output variables over the economic optimization horizon. For instance, figures 4.19 and 4.20 show the difference between the open- and closed-loop predictions for the reactant concentrations, temperature of the first reactor and temperature of coolant outlet in the second reactor for the first and fourth disturbance scenarios in table 4.2.

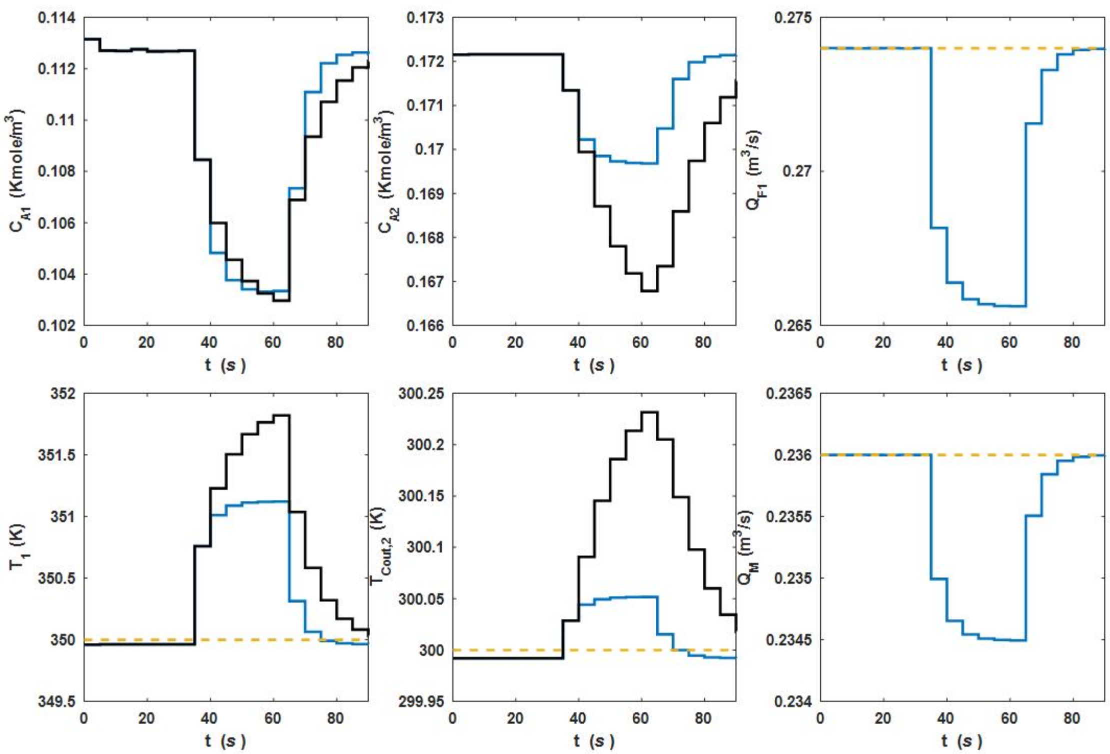

Figure 4.19: Closed- and open-loop predictions in the presence of first disturbance scenario. The closed-loop input and state variables (——), open-loop input-states (——), and the output constraints and nominal inputs of the open-loop system (- - -).

Table 4.11 shows the integral of the prediction error of the open-loop method comparing to the closed-loop prediction over the economic optimization horizon for the same order of the disturbance scenarios in table 4.2. The results show that prediction errors in the presence of disturbance in the coolant flow rate (scenarios 1, 2 and 4 in table 4.2) have

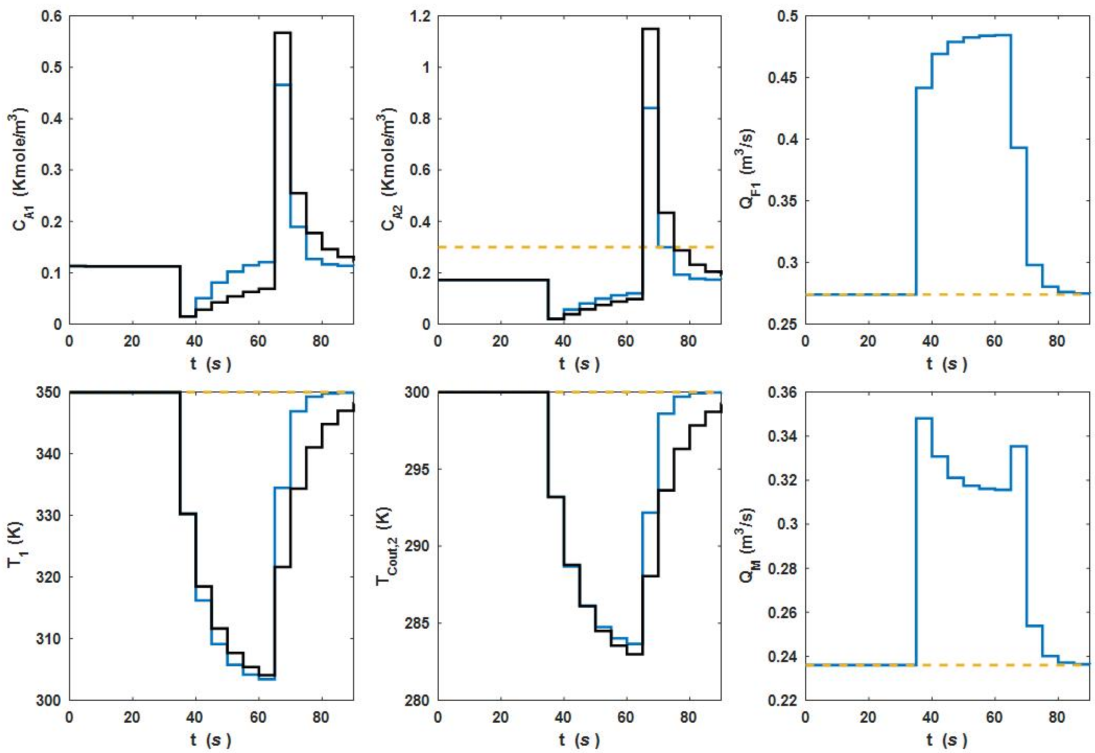

Figure 4.20: Closed- and open-loop predictions in the presence of fourth disturbance scenario. The closed-loop input and state variables (——), open-loop input-states (——), and the output constraints and nominal inputs of the open-loop system (- - -).

the same order of magnitude, whereas the prediction error of the open-loop model for the disturbance change in the feed concentration has a higher order of magnitude. Therefore, a significant difference in the performance is expected for the usage of closed-loop prediction in the DRTO system for the third disturbance scenario.

The open-loop results comparison of figures 4.19 and 4.20 reveals that the third disturbance scenario cause a larger deviation from the setpoint. Therefore, the MPC controller should provide a larger input action to regulate the system. The steady-state input-output gain for a step change in the disturbances could be calculated as a ratio of difference between the initial and final steady state over the percentage of change in the disturbance parameter. The steady state gains are shown in table 4.12. The disturbance to output gains for the

Table 4.11: Cumulative open-loop prediction error for different disturbance scenarios.

Disturbance scenarios	$e^2_{T_1}$	$e^2_{T_{c2out}}$	$e^2_{C_{A,2}}$
$+25\%$ short-term $Q_{c,1}$	4.652	0.3059	0.00009
-25% short-term $Q_{c,1}$	11.95	0.8184	0.00024
-95% short-term $C_{A,(F1\&M)}$	2208	300.90	0.64020
$+25\%$ sustained $Q_{c,1}$	8.670	0.5659	0.00016

change of the inlet feed concentration are significantly higher than that of the coolant flow change. This comparison of the steady state gains confirms the reason for the significantly different open- and closed-loop prediction in the presence of the large disturbance scenario.

Table 4.12: Steady state input-output gains for $Q_{c,1}$ and $C_{A,F1}\&C_{A,M}$ disturbances.

Input-output gains	$Q_{c,1}$ disturbance	$C_{A,F1}\&C_{A,M}$ disturbance
$\kappa_{T_{c2out}}$ $(K/\%)$	0.07	0.50
κ_{T_1} $(K/\%)$	0.01	0.17
$\kappa_{C_{A,F}}$ $(\frac{kmol}{m^3\%})$	2.20×10^{-4}	7.37×10^{-4}

4.2.6 Effect of the MPC Output Constraint on the Performance of CL-DRTO Formulation

As mentioned in section(3.4.1), the inclusion of hard output constraint in MPC formulation could result infeasible QP optimization problem in the presence of the unknown disturbances

(Zafiriou and Marchal [1991]). This problem could happen when there is no available input to move process output to the feasible region in the current MPC iteration step. A soft constraint formulation is considered for the MPC control layer of the dual-layer formulations to avoid infeasible QP optimization problem in the comparison study of the single- and dual-layer methods. However, for the unknown disturbance change in the fresh feed concentration, the EMPC formulation and the DRTO layer of the dual-layer methods result infeasible problem in the first update time after the disturbance changes. The infeasiblity occurs for the EMPC with the smallest update time and biggest update time at step 7, and 3 respectively. It also occurs for the OL- and CL-dual layer formulations at the third DRTO iteration step. The NLP problems which result from the economic optimization problem are solved using the fmincon MATLAB NLP solver with the interior point algorithm. When the problem is infeasible, fmincon attempts to minimize the value of constraint violation using the soft constraint formulation (MATLAB Optimization Toolbox [2014]).

In the original CL-DRTO-MPC formulation the output constraints are not considered in the embedded MPC subproblems of the CL-DRTO layer. The inclusion of the hard output constraints in the MPC subproblems of the closed-loop dual layer method adds more disjunctions. In other words, the hard constraint inclusion could cause infeasible QP subproblems, because in the intermediate iterations for the solution of the primary optimization problem, the optimization solver may attempt for the setpoint change scenarios which are not feasible for some of the individual MPC subproblems. In the case of the infeasible QP problem, the solution of previous iteration step for the MPC update time interval is used.

In order to show the effect of the output constraint inclusion in the embedded MPC subproblems of the CL-DRTO formulation, the same in-series CSTRs process and unknown disturbance scenarios are used. The CL-DRTO-MPC design parameters in table 4.6 are considered in the modified CL-DRTO formulation. The ARTs for the first to forth scenarios increase to $14.91s$, $13.28s$, $13.37s$, and $42.21s$ respectively, compared to the ART results of CL-DRTO formulation in tables 4.7, 4.8, 4.9, 4.10 . While the regulation and economic performances are similar to the case that there is no output constraint in the MPC subproblems, the computational effort increases which confirms that the QP subproblem results for some of the intermediate iterations are different in comparison to unconstrained MPC formulation. The increase in the ARTs also shows that in the CL-DRTO formulation, inclusion of the output constraints in the economic optimization layer is computationally more efficient than inclusion of them in the MPC subproblems.

The inclusion of soft constraint formulation in the MPC subproblems of the closed-loop dual layer formulation could potentially improve the regulation and economic performances when there is no feasible solution for the economic optimization problem. However, for the current case study problem, soft constraint inclusion only causes the increase in the average solution time of the last disturbance scenario. In this case the ART increases to $34.01s$ for the same reason which is discussed in the previous paragraph.

4.3 Chapter Summary

In this chapter the case study process, operating constraints and the optimization objective function are introduced. Also, different unknown disturbance scenarios and the plan of the comparison study for the chosen formulations are presented and discussed. In the results and discussion section design and tuning parameters are provided. Also, the methods and assumption in the implementation steps of each formulation are mentioned. Moreover, the expected computational results are qualitatively predicted for each method using the optimization problem size and the number of the economic and control problem iteration steps. The observations are reported for each disturbance scenario and the resulting economic, regulation and run-time criteria are compared and justified regarding the existing theories and previous results in the literature. The key points of this comparison study are highlighted in the conclusion chapter.

Chapter 5

Second Case Study Problem

5.1 Case study process: Linear MISO process model

In this chapter there is a brief description of the case study process which is followed by the definition of the operational constraints, and the economic objective of the optimal process operation. Also, the state space form of the model which is used in the MPC and real-time economic optimization, is presented. We also addressed the importance of choosing the case-study process, regarding the recycle effects in the linear systems and the extra degree of freedom due to the non-square form of the system. A process dynamics transition scenario in the product specification is considered for the performance comparison of the single- and two-layer methods. The implementation results of the chosen methods are interpreted and compared using the performance criteria.

5.1.1 Process description

A linear multi-input and single-output (MISO) process described as

$$y(s) = \frac{1}{750s^2 + 65s + 1} u_1(s) + \frac{1}{400s^2 + 40s + 1} u_2(s). \tag{5.1}$$

The output y responds to the input u_2 faster than u_1, and the cost of input u_2 is higher than that of input u_1. A rapid output transition could result higher revenue while it may result a higher production cost because of a higher contribution of the expensive resource u_2. Therefore, there must be a compromise between a rapid transition and an economic resource consumption. This case study problem is used by Jamaludin and Swartz [2015] for the performance comparison of the CL-DRTO and OL-DRTO formulation which could typically represent a linearized version of a chemical process. The linear nature of the model could be useful to provide a clear understanding of the observed input actions which result from different real-time operation strategies.

As mentioned in the introduction chapter, a process system with a material recycle might have some of the characteristics of the potential processes in which two-layer methods

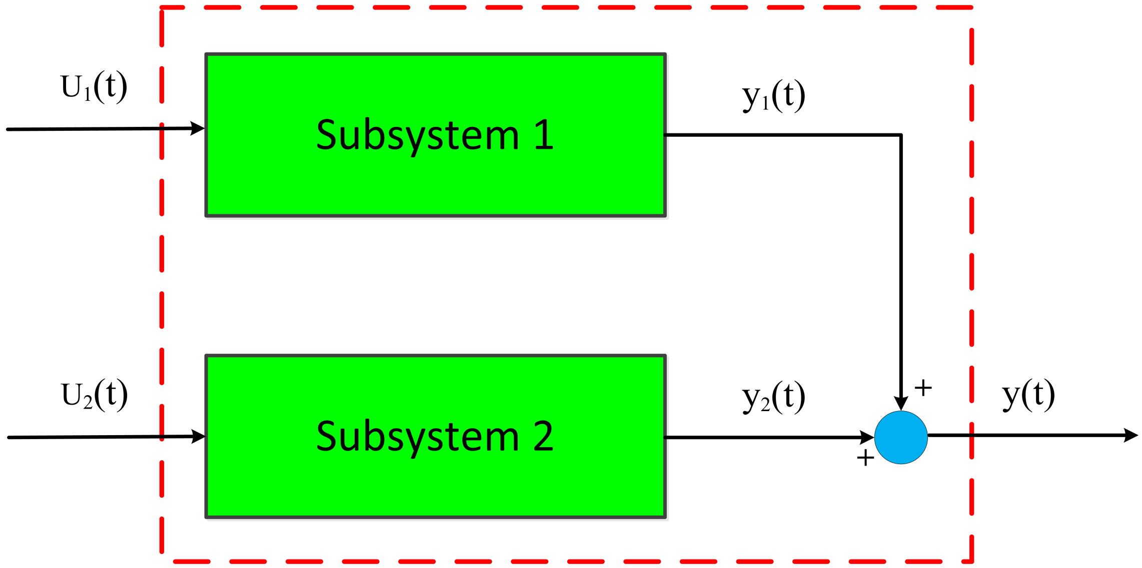

Figure 5.1: A linear multi-input and single-output case study problem.

may outperform the single-layer approach. A high ratio of the recycle stream could be considered in the design of the reaction-separation processes to maintain a low single-pass conversion to provide a high selectivity of the desired product. However, a high recycle to feed ratio generates two distinct time-scales for the transient behavior of the process dynamics (Luyben *et al.* [1999]). Moreover, a process with recycle stream can exhibit a severe steady-state snowball effect, which is a large variation in the process due to a small change in the feed conditions. This effect is undesirable because of limited processing capacity of the units such as liquid levels and turn-down ratio (Luyben [1994]). A regulatory controller could be necessary to prevent the large variations in the process. A sufficiently small controller sample time must be considered to react on the undesired process changes with both fast and slow time-scale. We believe that the transient effects of a system with recycle is a key point to determine which one of the single-layer and/ or two-layer methods could lead to a more efficient optimal process operation. For the study of the recycle effect subsystem 1 of figure 5.1 is designed to a recycle system of the two linear first-order models shown in figure 5.2.

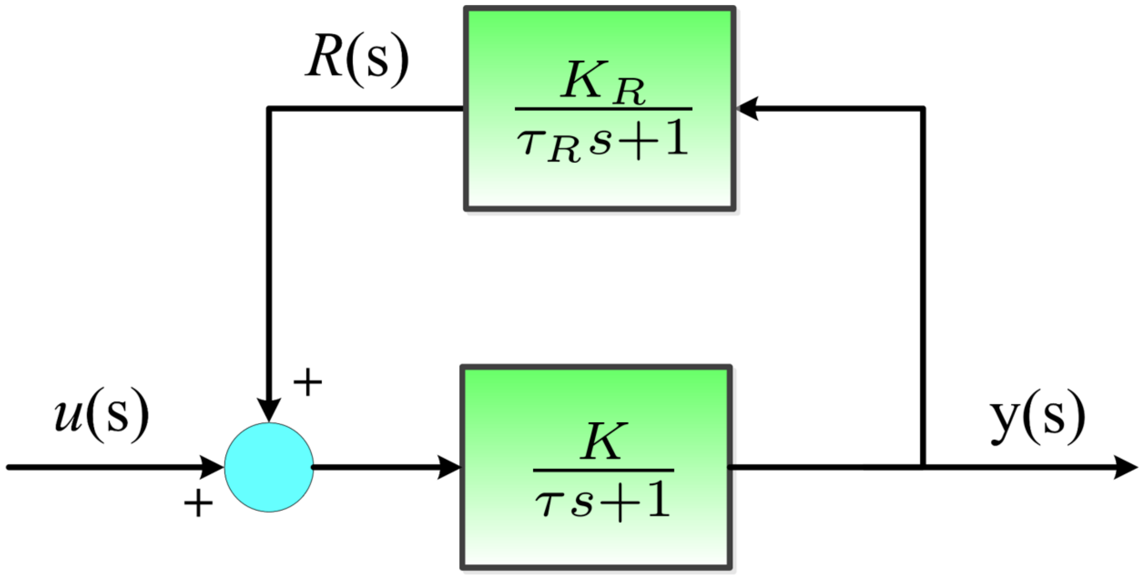

Figure 5.2: Simple open-loop process with recycle.

The equation describing the overall system is:

$$\frac{y(s)}{u(s)} = \frac{K(\tau_R s + 1)}{\tau \tau_R s^2 + (\tau + \tau_R)s + 1 - KK_R}. \tag{5.2}$$

Tosukhowong [2006] states that for many linear plant model with the material recycles stream, $0 < KK_R < 1$. Therefore the overall open-loop system has two negative real eigenvalues which means the system is stable. Increasing the steady-state recycle gain K_R, increases the process gain $(K/(1 - KK_R))$ which could be interpreted as an increase in the recycle to feed ratio. This change also increases the time constant of the second order system $(\frac{\tau\tau_R}{1-KK_R})^{(1/2)}$. This means that one of the time constants must become larger. Therefore an integrated plant with a material recycle displays a distinct slow and fast time-scale behavior. This behavior could be observed in a form of a fast initial response to a step change followed by a slow transient behavior. Baldea and Daoutidis [2007] propose a hierarchical controller framework for the systems with time-scale multiplicity due to the presence of material recycle streams. This approach might yield a superior computational, economic and control performance of the hierarchical methods in comparison to the single-layer method which does not take advantage of the time-scale multiplicity in a system. Different process gain and time constants are considered in section 5.7 which could reflect the effect of recycle gain K_R and time constant τ_R on the dynamic behavior of the case-study process. It is expected to observe from the performance analysis of the single-layer and dual-layer methods for the various process gain and time constants of the first subsystem that the two-layer methods could be preferable for the processes with recycle system.

The availability of two manipulated input variables for the optimal operation of a single output introduces an extra degree of freedom. In the linear case study of equation 5.1, the process output (y) is a linear combination of the input effects. This may lead to a clear understanding of the dynamic behavior of the system in response to the combination of the input actions. Therefore, in addition to the analysis of the effects of the recycle gain (K_R) on the performance of single- and dual layer methods, we will discuss the economic value of the manipulating inputs and address the condition that could possibly result better performance for the closed-loop DRTO in comparison to the EMPC approach.

5.1.2 The economic objective and constraints

Development of this case study process is motivated by a linearized model for the product grade transition problem. These types of problems are specifically used to conduct grade transition according to a-priori known schedules in the polymer and bioprocess industries. In the grade transition problem revenue is calculated only when the product quality is within an acceptable range. This means, when the quality does not meet a desired specification, it is not marketable. There is a demand only for the specific product grade that meets the quality constraints. This on-off switching mechanism in the economic objective could be approximated using a hyperbolic tangent function (Tousain [2002]). This continuous approximation technique is depicted in figure 5.3. This figure shows a typical transition from $y^{initial}$ to y^{target} in which R^1 and R^2 are the approximated switch functions of equation 5.3 to detect whether each point on the output trajectory is within the acceptable quality range or not. In this continuous approximation of revenue as a function of y, the desired product quality has a tolerance of $\pm\delta y^{target}$.

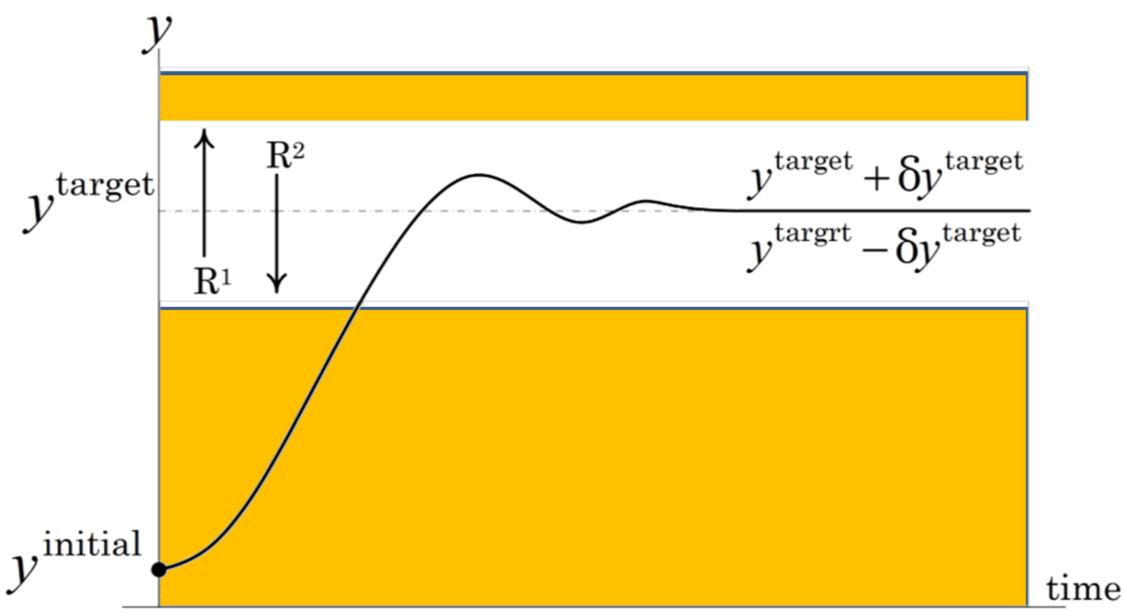

Figure 5.3: Continuous approximation of specification satisfaction using the hyperbolic tangent function.

$$
\begin{aligned}
R^1(y) &= \frac{1}{2}\tanh[\gamma(y - y^{target} + \delta y^{target})] + \frac{1}{2} \approx \begin{cases} 0, & y < y^{target} - \delta y^{target} \\ 1, & y > y^{target} - \delta y^{target} \end{cases}, \\
R^2(y) &= \frac{1}{2}\tanh[\gamma(y^{target} + \delta y^{target} - y)] + \frac{1}{2} \approx \begin{cases} 1, & y < y^{target} + \delta y^{target} \\ 0, & y > y^{target} + \delta y^{target} \end{cases}.
\end{aligned} \tag{5.3}
$$

where γ is a tuning parameter used to define the steepness of the switching function. $R^1(y)$ is responsible for the detection of minimum quality bound violation and $R^2(y)$ tracks constraint violation for the maximum quality bound. Multiplication of product revenue term by R^1R^2 results in a revenue contribution if the product is within the specification limits. Also, it should be noted that an inefficient tuning parameter could cause numerical problems which could possibly result a suboptimal solution (Lam [2006]). The economic objective is formulated in equation 5.4 to maximize the net profit value which is by the standard definition in the form of subtraction of cost from the revenue over the economic optimization horizon:

$$min\ \Delta t_{MPC} \sum_{j=0}^{N-1} w_{U1}u_{1,j} + w_{U2}u_{2,j} - w_y R^1(y_{j+1}) R^2(y_{j+1}). \tag{5.4}$$

The control vectors are discretized based on the MPC sample time of Δt_{MPC} and R^1 and R^2 are evaluated with a sample time equal to that of the control vector discretization. The nominal unit prices w_y, w_{U1}, and w_{U2} corresponding to the output and input variables, the MPC design parameters, and tuning parameters are summarized in table 5.1.

The manipulated variables, output variables and the set-points are constrained as follows:

$$\begin{aligned} 0 \leq y^{Ref} &\leq 1.1, \\ 0 \leq u_2^{Ref} &\leq 1.5, \\ 0 \leq y &\leq 1.1, \\ 0 \leq u_1 &\leq 1.5, \\ 0 \leq u_2 &\leq 1.5\ . \end{aligned} \tag{5.5}$$

5.2 Solution strategies

In this study, we employ the sequential approach to solve the dynamic optimization problem in the economic optimization step of the open-loop two-layer and single-layer method. In the sequential method, only the control vector variables are discretized. Then a dynamic process model in each function evaluation of the economic optimization is solved using the values of the discretized control variables. In the sequential implementation approach of the closed-loop two-layer DRTO formulation a sequence of convex QP sub-problem and ODE model are paired and solved for each function evaluation of the economic optimization problem. Each pair of the convex QP and ODE arises from a sequence of MPC sub-problem calculations and the implementation of the control action to the model of the DRTO layer.

Since, all QP problems in the dual-layer methods are convex, the QP solvers efficiently solve the QP problems to their global minimum. Most of the MPC formulations use a discrete state-space model to convert MPC optimization problems to the standard QP form which is defined in the QP solver packages (for e.g. See Rawlings and Mayne [2009]). The frequency domain model of the case study problem must be transformed to a time-domain model and be discretized to be converted to the desired form of the model. The dynamic model which is describing the systems behaviour is converted to the following observable state-space form in MATLAB:

$$
\begin{aligned}
\frac{dx}{dt} &= Ax + Bu, \\
y &= cx, \\
A &= \begin{bmatrix} -0.0748 & 0.0774 & -0.0200 & 0.0134 \\ -0.0065 & -0.0166 & -0.0248 & -0.0069 \\ 0.0000 & 0.0140 & -0.0952 & -0.0390 \\ 0.0000 & 0.0000 & 0.0434 & 0.0000 \end{bmatrix}, \\
B &= \begin{bmatrix} -0.0891 & 0.1330 \\ 0.0458 & -0.0684 \\ 0.0748 & 0.2003 \\ 0.0000 & 0.0000 \end{bmatrix}, \\
c &= \begin{bmatrix} 0 & 0 & 0 & 0.2876 \end{bmatrix}.
\end{aligned}
\tag{5.6}
$$

This state-space model is discretized in MATLAB based on the controller sample time for implementation in the DRTO-MPC and EMPC formulations. Since input u_2 has a significant impact on the transition dynamics and the overall process economics, we include it as a manipulated variable with a set-point trajectory, in addition to the set-point for output y in the two layer methods.

Manipulated input constraints in the MPC optimization problem and the economic optimization problems in both of the single-layer and dual-layer methods are considered as a hard constraint formulation. However, in the dual-layer methods the output constraints

Table 5.1: Nominal unit price, design parameters and tuning parameters for the implementation of the single-layer and dual layer formulations.

Unit prices & Design parameters	Tuning parameters
$w_y = 100$, $w_{U1} = 2$, and $w_{U2} = 10$	MPC output tracking weight $Q = 1$
MPC prediction horizon $p = 30$	MPC move suppression weight $R = diag(1, 1)$
MPC control horizon $m = 3$	Control tracking weight $S = diag(0, 1)$
MPC update time $\Delta t_{MPC} = 2min$	Switch function steepness tuning parameter $\gamma = 8$
DRTO update time $\Delta t_{DRTO} = 20min$	Economic optimization horizon $N = 3$, 6, 20, 30, 40, & 50
EMPC update time, $\Delta t_{EMPC} = 2min$	Control effort penalty tuning parameter $\rho = 20$

are not considered in the MPC optimization problems due to the robustness and stability issues (Zafiriou and Marchal [1991]). Therefore, the output constraints must be considered in the economic optimization problems in the closed-loop formulation. Also the appropriate adjustment of the set-point trajectories in the dual-layer method would indirectly compensate for the output constraints in the regulatory level. The ODE models in the economic optimization problems are solved using ode45, MATLAB's built-in solver, and the MPC optimization problems are solved using quadprog, MATLABs QP solver, with the interior-point algorithm. The NLP problems which result from the economic optimization problem are solved using the fmincon MATLAB NLP solver with the interior point algorithm. A warm start strategy using the solution of the previous NLP optimization problem is used to initialize the input variables. Computations are performed in MATLAB a2014, using a 3.4 GHz INTEL CORE-i7 with 16 GB RAM running Windows 8.

5.3 Validation of the results for the two-layer DRTO formulations

There is a very high possibility that the NLP optimization problems which may arise from the discretization of the economic optimization problems in either the single-layer and/ or dual layer methods are non-convex and have a local optimal solution. Moreover, because of the inherent non-smoothness in the structure of bi-level or in general a multi-level optimization problem, gradient based optimization methods might have some issues such as convergence failure problem and/ or converging to the local optima (Clark and Westerberg [1983]). Therefore, we decided to validate our results for the OL-DRTO-MPC and the rigorous CL-DRTO-MPC with the results of the simultaneous implementation approach for the same problem formulation. This performance check has been conducted for some of different tuning parameters which are mentioned in Jamaludin and Swartz [2015], and Jamaludin and Swartz [2016]. Figure 5.4 shows the resulting set-point changes and the input-output behavior of the system for the OL-DRTO with a control horizon of $m = 20$ for the sequential implementation approach. The input U_2 and output y changes in this figure are the same as those of the corresponding plots for the simultaneous solution method in the reference. In this figure, dynamic changes for all internal state variables and the first input are displayed to make sure that there is no internal instability. Because of the observable form of the model, dynamic changes of x_4 would be a scaled version of y, therefore there is no need to display x_4.

Also, the simulation result for the CL-DRTO formulation with the same tuning parameters in Jamaludin and Swartz [2016] is shown in figure 5.5. The U_2 and y trajectories are the same as those in the reference. Also, the optimal value of the economic objective function, is equal to $\Phi_{eco} = 7385\$$ which is very close to that of the simultaneous solution for the rigorous CL-DRTO-MPC formulation ($\Phi_{eco} = 7371\$$).

In the simultaneous implementation of the CL-DRTO formulation the necessary and sufficient KKT conditions which are equivalent to the solution of each MPC QP problem are substituted in the primary optimization problem to convert the multi-level rigorous formula-

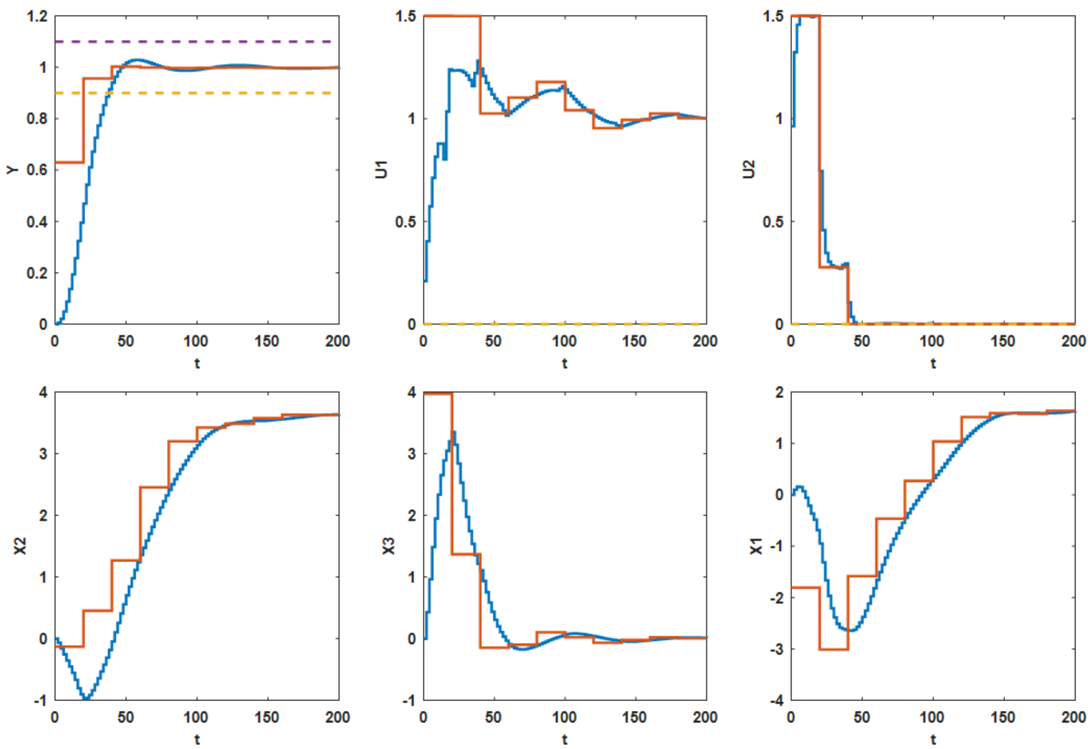

Figure 5.4: OL-DRTO inputs and output responses and internal dynamics of the system for the MPC control horizon $m = 20$. The input, output, and state variables (——), optimal reference signals (——), and the output constraints (- - -).

tion, and its hybrid and bi-level approximation of the problem to a single-level optimization problem. In this approach the non-smoothness characteristic of the multi-level optimization problem appears in the form of the complementarity constraints. These constraints take the form $\eta_i \mu_i = 0$, and are generally hard to solve due to violation of constraint qualifications in the nonlinear programming (NLP) problem (Baumrucker *et al.* [2008]). The MPCC could be reformulated as a continuous approximation of the switching behavior of the complementarity constraints using relaxation methods, exact penalty method and/ or a mixed-integer approach (Lam *et al.* [2007], and Soliman *et al.* [2008]). If the saturation pattern, i.e., which bounds are active at which time steps, were known before solving the MPCC problem, the inclusion of the complementarity constraints in the form of $\eta_i \mu_i = 0$

could be avoided. Therefore, it is also possible to use partitioning heuristics technique to estimate the input saturation which could eliminate the complementarity constraints (Li and Marlin [2011]). The partitioning idea is to solve the problem assuming no input bounds are active. In the next step the active-set is updated according to the solution of the unsaturated inputs which have a value larger than the limits. In this method the unbounded version of the problem must be solved for a number of iterations. However, Clark and Westerberg have shown that the simultaneous solution technique which uses the embedded KKT condition of the inner problem and solves a series of single-level NLP problem for different complementarity constraint relaxation parameter is computationally more efficient than the partitioning heuristic method. In the constraint relaxation approach, the resulting NLP problems including the embedded KKT conditions should be solved several times to find the proper relaxation parameter. However, in the exact penalty reformulation approach with a pre-tuned penalty parameter ($\rho > \rho_c$), the NLP problem is solved one time (Jamaludin and Swartz [2016]). In this method the complementarity constraints of the form $\eta_i \mu_i = 0$ are moved from the constraint set of the MPCC problem to the objective function as an additional penalty term ($\rho \Sigma \eta_i \mu_i$) with a penalty parameter ρ. This reformulation method leads to an NLP problem which could be solved using a standard NLP solver. This method needs a sufficiently large penalty parameter ρ to satisfy the complementarity constraint. Choosing ρ too large may cause longer solution times and numerical problems. In the sequential implementation approach there is no complementarity constraint formulation. Thus, this method does not require relaxation and/ or complementarity penalty parameter tuning. Also, it is easier to set up the problem in the sequential solution approach. In this method, the interior-point NLP the inner problems are treated as a black box in the function evaluation of the primary optimization problem and the gradients are approximated using the finite difference method. Therefore for the effective implementation, we believe that the solution of the inner problem should be computationally reliable and cheap to achieve a better solution flow in comparison to the simultaneous solution method. In our CL-DRTO formulation all of the inner problems are QP which guarantees the global solution of them due to convexity of the QP. Thus the QP problems could be solved computationally reliably and efficiently using the quadprog solver in MATLAB.

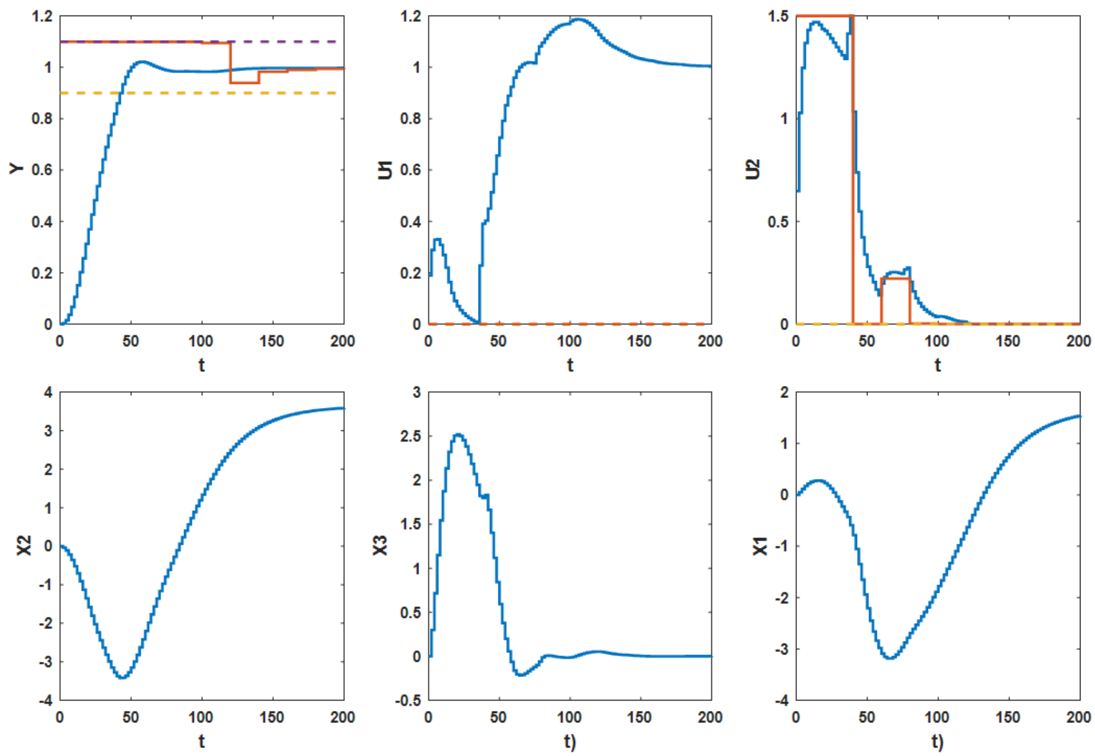

Figure 5.5: Closed-loop response of output y and inputs u_1, and u_2 and dynamic behavior of the internal state vaiables for $N = 150$. The input, output, and state variables (——), optimal reference signals (——), and the output constraints (- - -).

In the sequential method the inner QP problems are accurately solved in each function evaluation of the primary optimization problem, while in the MPCC each set of KKT optimality conditions with the penalty and/ or relaxation parameter represents an approximate solution to the corresponding original QP sub-problem, although high accuracies are attainable with a suitable penalty parameter and convergence tolerance. Our results show that both of simultaneous and sequential methods could converge to the same solution for an appropriate starting point.

5.4 OL- and CL-DRTO performance comparison for the de-tuning effects of the p

Model predictive controllers are 'tuned' by adjusting parameters such as the prediction horizon, and weights in the quadratic regulatory performance criterion (Maciejowski [2002]). However, if the objective of increasing robustness is sought the performance could be improved by de-tuning of the MPC. Jamaludin and Swartz [2015] have studied the de-tuning effects of the move suppression weights and the MPC control horizon on the economic performance of the OL- and CL-DRTO formulation. They showed that the CL-DRTO formulation could effectively account for the MPC controller tracking capability. This capability is particularly effective in the cases where the MPC controller is detuned for robustness purposes. By contrast, the economic optimization problem of the OL-DRTO formulation is unaware of the MPC controller detuning, hence causing a sluggish process transition and a lower economic return.

A sufficiently large prediction horizon would ensure the closed-loop stability of the MPC-plant system for open-loop stable systems without any terminal constraint (Maciejowski [2002]). In this study we show that considering a larger MPC prediction horizon is also equivalent to the DRTO-MPC detuning, in a sense that the economic performance would decrease with an increase in the prediction horizon length (figure 5.6). A large prediction incurs a deterioration in economic performance because the controller would not achieve a prompt tracking of the changes in the output set-point for a long sequence of output using a fixed number of input moves in each MPC step. Figure 5.6 also shows a similar pattern of this behavior for the open-loop DRTO formulation which occurs for the same reason. It is important to point out that the economic return of the OL-DRTO horizon is still lower than that of the CL-DRTO-MPC for the larger MPC prediction horizon. The reason for this lower economic performance is that the OL-DRTO economic optimization layer does not account for the effect of the limited MPC control input moves over the large MPC prediction horizon. Therefore the OL-DRTO-MPC would prefer to use the more effective yet more expensive manipulating input resource U_2. By contrast, the closed-loop counterpart is aware of the next MPC control actions and demands a lower U_2 usage by reducing the U_2 set point.

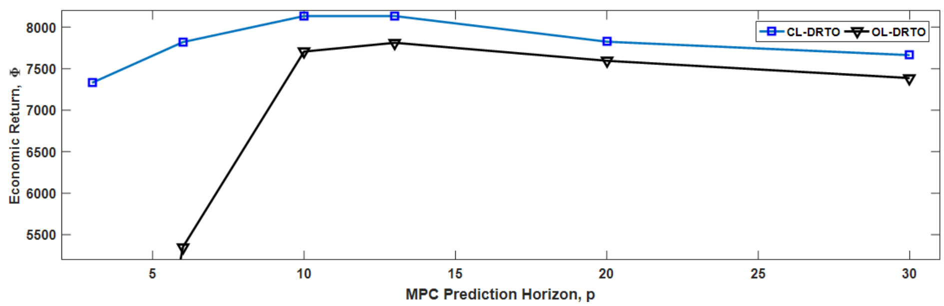

Figure 5.6: Effects of the MPC prediction horizon on the economic performance of the OL- & CL-DRTO.

Figure 5.6 clearly shows how a prediction horizon smaller than $p = 10$ would drastically reduce the economic improvement of the OL-DRTO-MPC at the expense of maintaining the stability. An inference of this behavior could be drawn by comparing the input-output changes of the case study system for prediction horizons ($p = 6$, and 20) in figure 5.7 and figure 5.8. In the simulation result of figure 5.7 the MPC prediction horizon is too short, so that the controller is short-sighted. Thus, the MPC does not respond early enough to result a rapid output transition. In this case study, the MPC changes the first input U_1 too slowly and mostly relies on the more expensive U_2, because of the fast U_2 input-output response. In contrast, for the larger prediction horizon $p = 20$, the MPC predicts the slower U_1 input-output effect over a larger time span, so it could respond for the set point tracking early enough using the cheaper control action to obtain a rapid transition. This effect could also lead to an economic usage of U_2 which merely contributes in the early stage of transition for the purpose of a faster transition.

A moderate form of the economic loss is observed in the performance of the CL-DRTO-MPC for the MPC prediction horizon smaller than $p = 10$. This is due to the fact that the economic optimization layer of the CL-DRTO-MPC inherits the tracking capability of a sequence of the short-sighted MPC steps over an economic horizon which is significantly larger than the prediction horizon of each individual MPC step. This inherited property allows the economic optimization layer to confront the poor stability property of the MPCs. A detailed observation of the input-output set point changes in figure 5.9 and figure 5.7 shows that the CL-DRTO provides larger and more active set point changes exploiting the collective predictions and tracking effects of the sequence of MPC controllers. This set point adjustment leads to a timely response of U_1 which improves the economic performance of the system to an appreciable extent. Figure 5.6 shows that for $p = 6$ and $p = 20$ CL-DRTO-MPC results approximately the same economic performance. However, figure 5.9 and figure 5.10 show that there are less set-point moves for the CL-DRTO-MPC system with a larger MPC prediction horizon to obtain the same economic performance.

In our performance comparison, an equal economic input move and prediction horizon is considered in the EMPC formulation for the reason of consistency with the economic layer of the dual-layer methods. Thus, a similar detuning behavior in the economic performance of the single-layer method is not expected because of the equal EMPC prediction and control horizon. The EMPC horizon and update time effects will be explored in the next sections which helps to establish the basic foundation for the single- and dual-layer performance comparison.

5.5 Horizon length and update time effects on the performance of the EMPC

Lao *et al.* [2014] discuss that the economic performance benefit of EMPC over conventional tracking MPC may strongly depend on the horizon length of the economic optimization. A large EMPC horizon severely increases the number of the decision variables in the resulting NLP problem in each EMPC step. The large NLP problem size increases the solution time, which may cause difficulty for real-time applications especially for large-scale problems.

In this situation the economic optimization problem could be solved less frequently (i.e., for a large economic update time) for the sufficiently large economic horizon to determine the set point. Then the economically optimal set points are passed to the MPC control

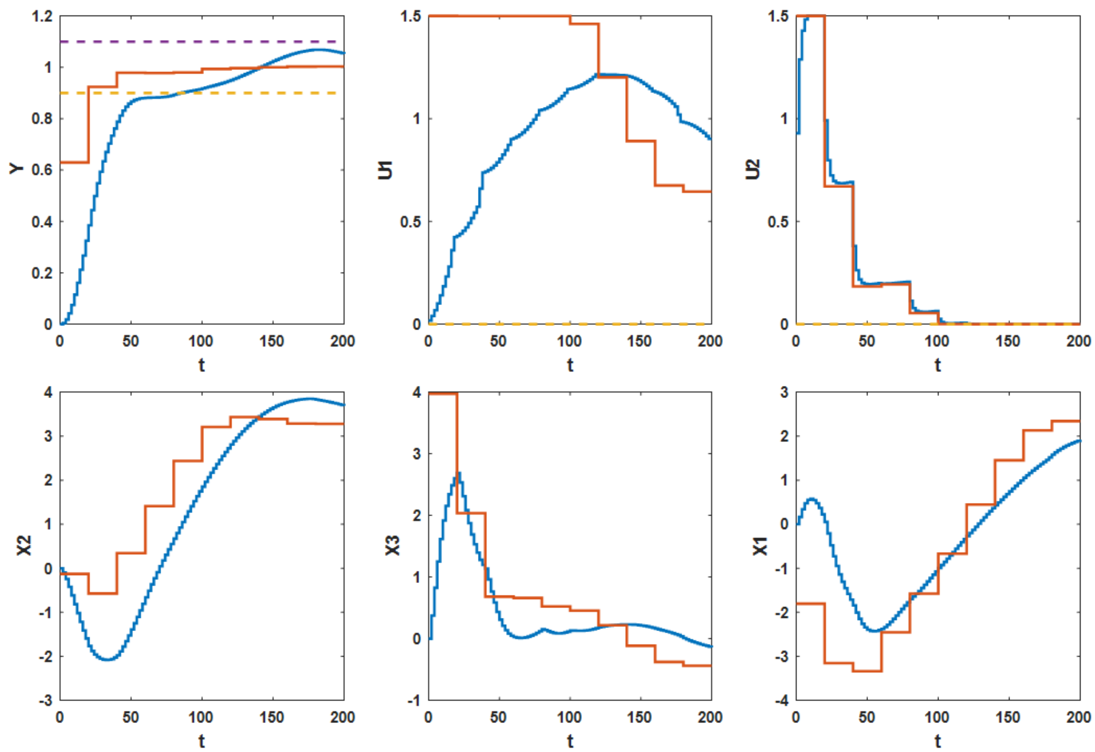

Figure 5.7: OL-DRTO inputs and output responses and internal dynamics of the system for the MPC prediction horizon $p = 6$. The input, output, and state variables (——), optimal reference signals (——), and the output constraints (- - -).

layer which solves a QP optimization problem for each MPC step in a suitably short time to track the optimal set-point until the next economic optimization update time. This strategy could also decrease the overall computational burden compared to the application of the EMPC. In this section, the EMPC horizon length effect is investigated for the EMPC with the update time equal to that of the MPC in the dual-layer formulations. An increase in the EMPC horizon length form $N = 2$ to 6 improves the economic return (Φ_{eco}) from 7815.0 to 7866.0\$ while the average solution for each EMPC step increases from 1.38 to 4.31s. However, the economic return remains approximately the same by an increase in N from 6 to 30 and the average solution time of each EMPC step increases to 146.21s. A desired economic improvement is notable for the optimal economic return ($\Phi_{eco} = 8050.51\$$)

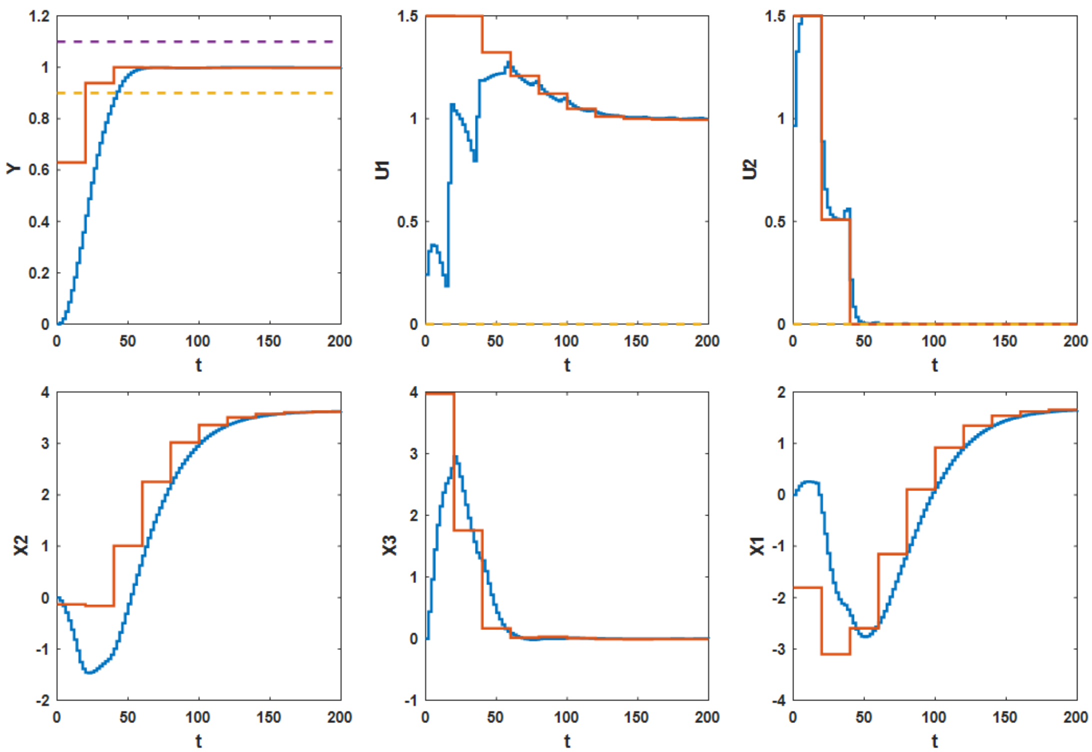

Figure 5.8: OL-DRTO for $p = 20$.

by increasing N from 30 to 40 for the average solution time of 307.2s, which is too high for the online implementation. There is a possibility to increase the EMPC update time for the same length of the economic optimization horizon to reduce the computational burden for the online application of EMPC with the large horizon length. For the increasing sequence of the economic update times $T_e = 2$, 4, and 8, following economic values of $\Phi_{eco} = 8050.51$, 8047.01, and 8003.81\$ are obtained for the average run time $ART = 307.2$, 117.31, and 11.66s, respectively. This result means that the effect of the EMPC update time is negligible in comparison to the horizon length effect on the economic performance.

Ochoa *et al.* [2010] claim that in the dead period between the large update time in the single-layer method, there is no feedback to compensate for the undesired effects of the unknown disturbance and/ or uncertainties. Simulation results of figure 5.11 for $T_e = 8$ and $N = 12$ shows output quality constraint violation. This constraint violation demonstrates

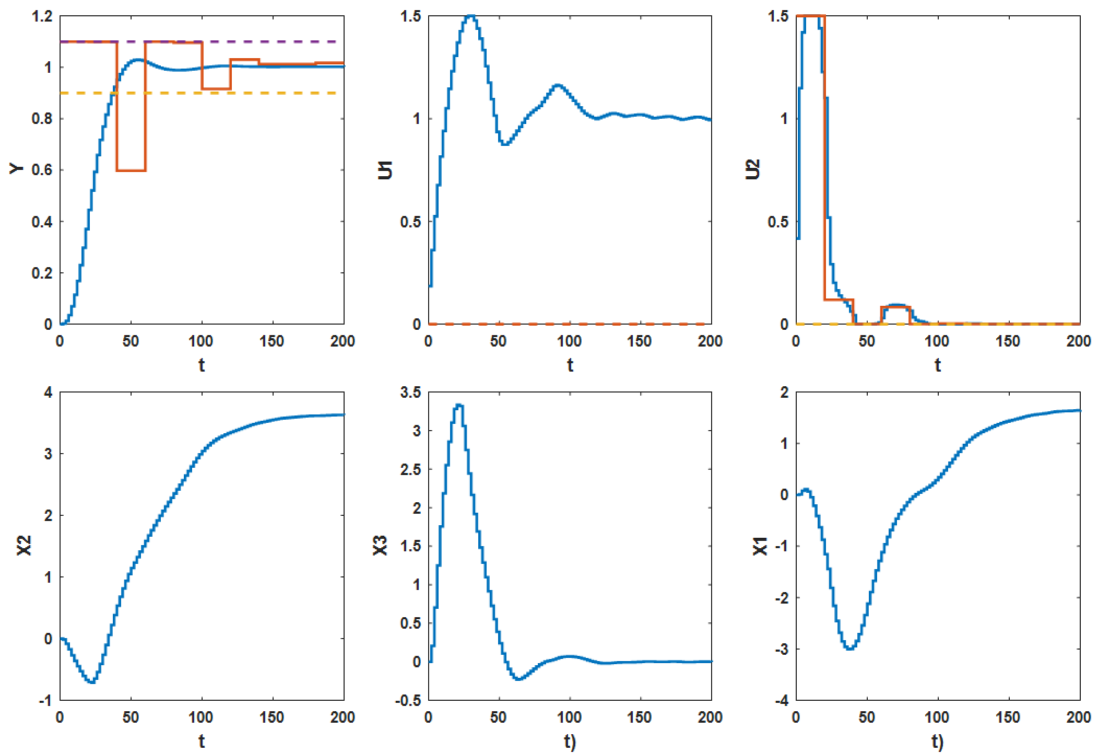

Figure 5.9: CL-DRTO inputs and output responses and internal dynamics of the system for the MPC prediction horizon $p = 6$. The input, output, and state variables (——), optimal reference signals (——), and the output constraints (- - -).

that the EMPC may perform an unsatisfactory regulation function due to the insufficient horizon length of $N = 12$, even when there is no unknown disturbance and/ or uncertainty. However, for the same update time a larger horizon would resolve the issue which is shown in figure 5.12. This result shows that EMPC with a large update time and insufficient horizon length could suffer from unstable behavior. Due to the short economic horizon length, EMPC cannot capture the effect of control input for a sufficiently long future predictions. Therefore, the EMPC attempts to improve the economic return without being aware of the possible consequences of its current action. Thus, it drives the plant into 'dead-ends' from which there is no feasible solution which could prevent the output from escaping the acceptable quality bound. This issue motivates consideration of a sufficiently large EMPC

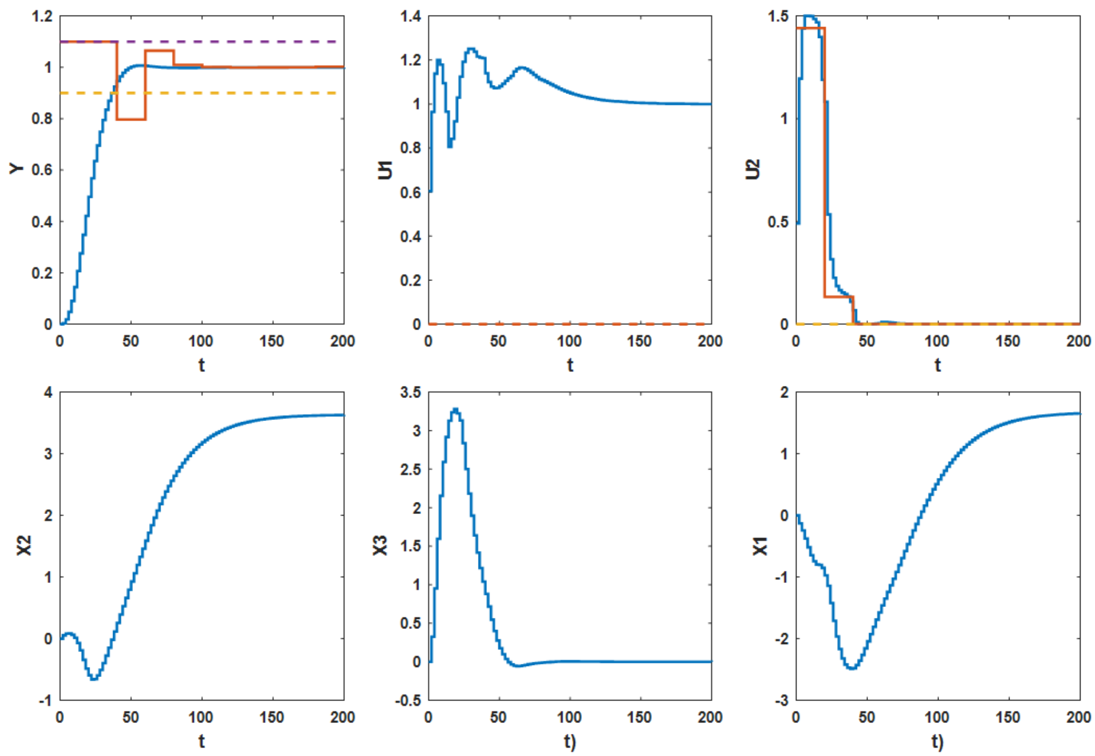

Figure 5.10: CL-DRTO inputs and output responses and internal dynamics of the system for the MPC prediction horizon $p = 20$. The input, output, and state variables (——), optimal reference signals (——), and the output constraints (- - -).

horizon N, to minimize the risk of economic performance loss and the output constraint violation.

Similar to the smooth input changes in the MPC simulation results, smooth input changes in the EMPC simulation results could reflect the desired detuning effect. The EMPC formulation which is used for the application of the optimal transition of the process output may potentially demand a large input change and may use the maximum available control action to carry out a fast dynamic transition. Therefore, the EMPC acts aggressively by a sharp increase of U_1 to the maximum available control action (figure 5.12) which results a higher overall control effort (OCE) in comparison to that of the dual-layer method in figure 5.8). The OCE is defined in equation 5.7:

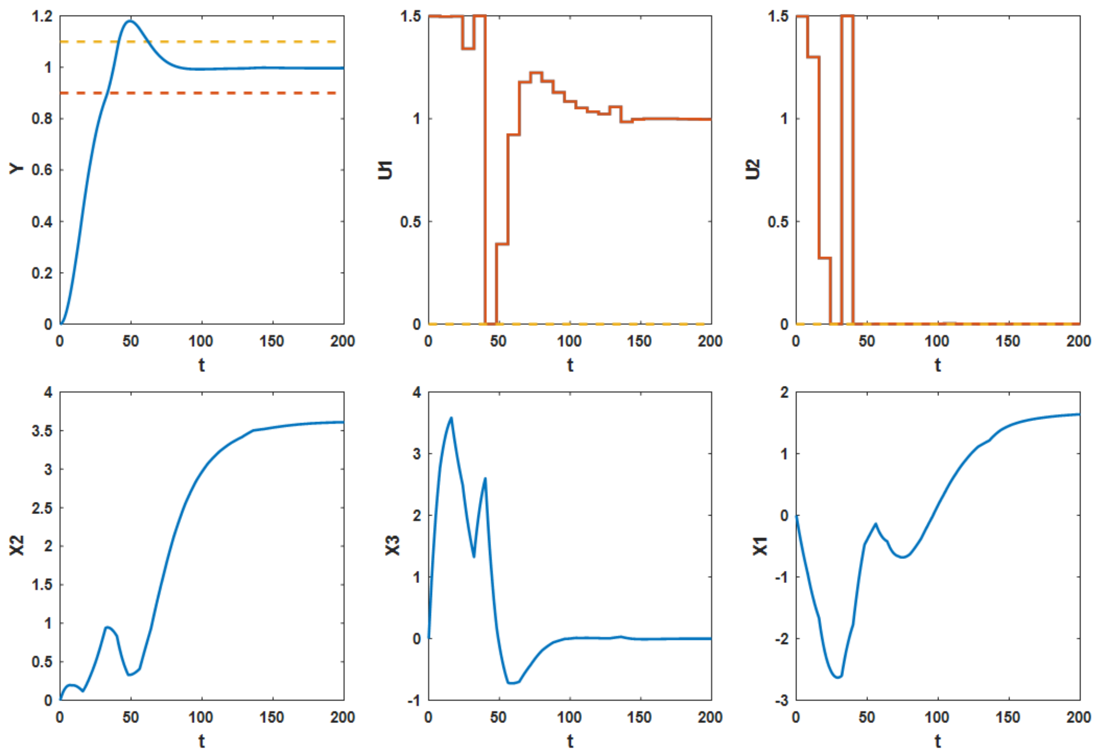

Figure 5.11: EMPC with $T_e = 8$ & short horizon $N = 12$.

$$OCE = \sum_{j=0}^{j_{max}-1} \Delta U^T R^{MPC} \Delta U,$$
$$j = (t_j - t_{initial})/T_c, \quad t_j \in [t_{initial}, t_{final}]\,. \tag{5.7}$$

where R^{MPC} is equal to the move suppression weight of the MPC control layer in the OL- and CL-DRTO-MPC formulation. The update time instances, t_j are the EMPC and/ or the MPC update time over the simulation time and ΔU is the optimal input change which is applied to the system at time t_j. The OCE could be determined for the EMPC and the dual-layer methods for the quantitative representation of the overall control effort of the single-layer and two-layer methods. For the EMPC performance result OCE varies in the range of $4.8 - 7.5$ depending on the value of the update time and the horizon length. The OCE value for the CL-DRTO-MPC formulation is in the range $1.46 - 2.11$ and for the

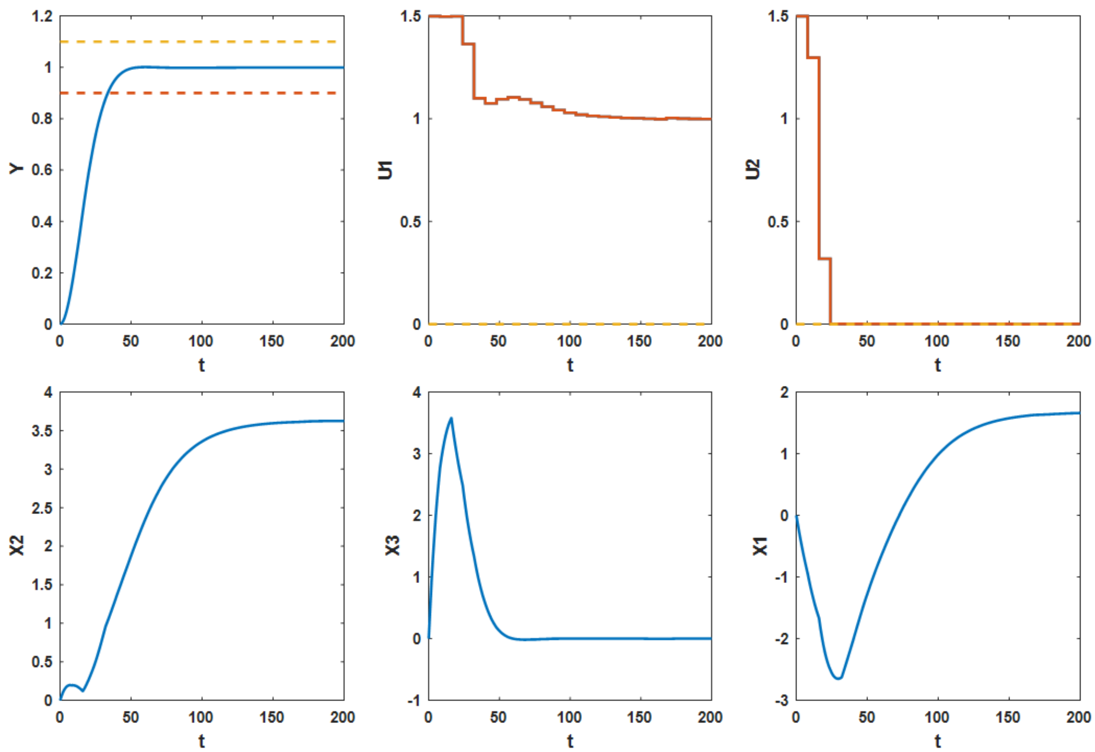

Figure 5.12: EMPC with $T_e = 8$ and horizon:20.

OL-DRTO is in the range of $2.07 - 2.30$ in which the lower ranges correspond with the MPC prediction horizon of $p = 30$. The OCE value of the EMPC is 2 to 5 times greater than that of the dual-layer methods. This indicates that the EMPC formulation performs aggressive input changes, while figure 5.6 shows that the CL-DRTO-MPC with an aggressive MPC prediction horizon $p = 13$ achieves approximately the same economic performance using less control effort of $OCE = 2.11$.

5.6 The EMPC, OL- and CL-DRTO-MPC performance comparison

A quadratic penalty term for the control inputs moves similar to that of the tracking MPC could be considered in the EMPC objective function (Amrit *et al.* [2013]). The economic performance results of the EMPC for different horizon length are obtained for the hybrid EMPC objective function. This hybrid EMPC objective function is a summation of the net profit term and the control effort penalty term $\Sigma \Delta U^T R^{MPC} \Delta U$ with the tuning weight of $\rho = 20$ over the economic optimization horizon. This control effort penalty weight ρ is tuned such that the OCE is in the range of the OCE for the OL- and CL-DRTO-MPC formulations. Also, average run time (ART) is considered for the EMPC and dual-layer methods. The average of the NLP problem solution time for the EMPC formulation and the summation of the averaged NLP and QPs' solution times for the dual-layer methods are considered as ART criterion. For the purpose of comparison, in all of the formulations the ART is calculated for a fixed time interval that is equal to the DRTO update time. The ART, OCE, and economic performance results are shown in table 5.2. Figure 5.15 Shows that the EMPC with a short horizon of $N = 3$ tends to increase the first input U_1 from the early EMPC steps, because the prediction horizon length is not long enough to acquire the knowledge of the fast U_2 input-output behavior. Moreover, the use of a higher U_2 input action is apparently an expensive option from the point of view of the short-sighted EMPC. Therefore, the EMPC starts with a U_2 input action close to 1. By contrast, because of the longer optimization horizon the CL-DRTO-MPC is aware of the fact that a temporarily high U_2 input action suffices to raise the output to the desired grade interval. Figure 5.13 shows the simulation results for the CL-DRTO-MPC formulation with economic optimization horizon $N = 30$. As a consequence of a large U_2 action, the CL-DRTO-MPC performs a maneuver to reduce the cost for the use of the unnecessary U_1 input actions over a H_2 period of time, which is shown in figure 5.16. Also, this figure qualitatively shows that the cumulative U_1 input resource usage of the CL-DRTO-MPC is less than that of the EMPC with the short horizon. In other words, the CL-DRTO-MPC formulation finds a solution which is a compromise between the costs of the more effective yet more expensive input U_2 and the less effective and cheaper U_1 input resource.

Table 5.2: Economic, computational and control move performance of the single- and dual-layer methods.

economic optimization horizon	Economic objective ($)	ART	Overall Control effort
EMPC $N = 3$	$\Phi_{eco} = 7169.01$	14.92	$OCE = 1.86$
EMPC $N = 6$	$\Phi_{eco} = 7285.00$	45.44	$OCE = 1.85$
EMPC $N = 10$	$\Phi_{eco} = 7328.11$	113.22	$OCE = 1.86$
EMPC $N = 20$	$\Phi_{eco} = 7375.00$	375.83	$OCE = 1.88$
OL-DRTO-MPC $N = 30$	$\Phi_{eco} = 7387.00$	2.48	$OCE = 2.07$
CL-DRTO-MPC $N = 30$	$\Phi_{eco} = 7663.60$	13.74	$OCE = 1.46$
EMPC $N = 30$	$\Phi_{eco} = 7730.04$	10.97*	$OCE = 1.95$
EMPC $N = 50$	$\Phi_{eco} = 7766.30$	12.21**	$OCE = 2.2$

* & ** (These ART are calculated for $T_e = 10$ and the equivalent economic horizons.)

An equal input unit price for U_1 and U_2 intuitively means that the single- and dual-layer economic optimization methods may often prefer to use U_2 which has a faster input-output effect compared to that of U_1. The manipulated input preference of the economic optimizers suggest that the inputs should essentially have distinct unit prices to exhibit the input compromise which is seen in the application of the CL-DRTO-MPC formulation. Also, observation of this behavior is only expected for the case study problems in which the unit price of the input resource with a faster input-output response is higher than that of the input resource with a slower input-output changes. Otherwise, the economic optimizer would obviously prefer to use the effectively fast and cheap input resource to minimize the input cost. Moreover, an extremely large difference in the unit price virtually means that do not use the extremely expensive manipulated input option.

The economic performance of the OL-DRTO-MPC with the smallest average run time

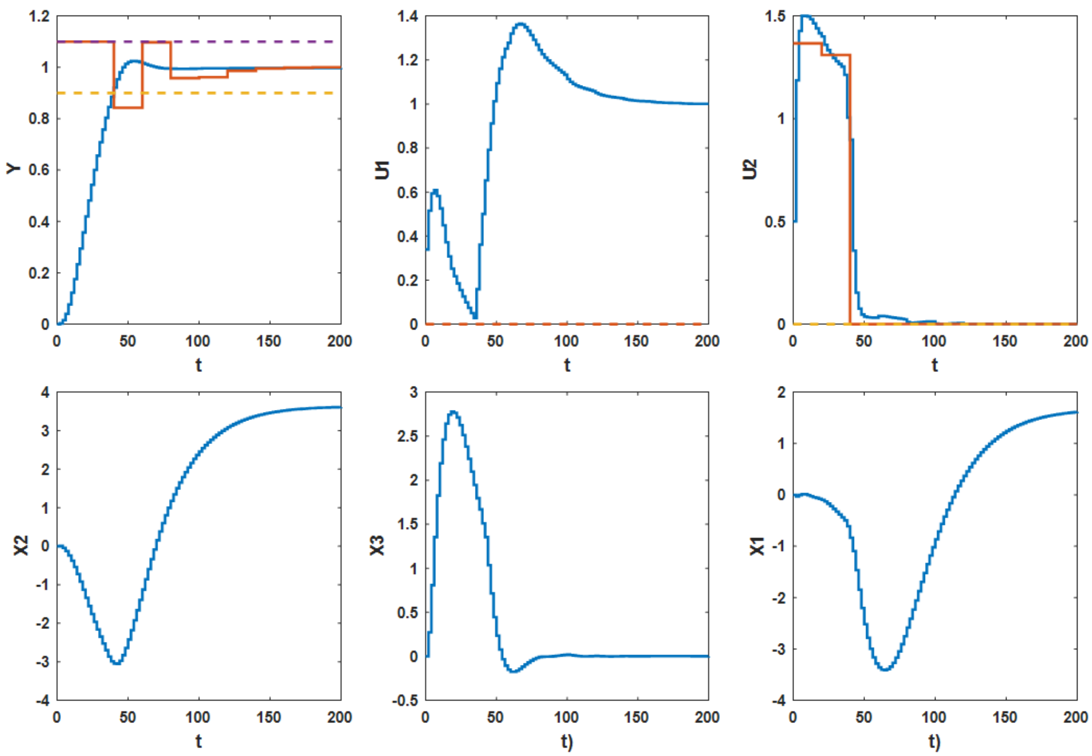

Figure 5.13: Closed-loop DRTO results for $N = 30$.

(ART) is slightly higher than that of the EMPC with the short horizons. A longer economic horizon of the OL-DRTO could be a possible reason for the higher economic performance of OL-DRTO-MPC in comparison to the EMPC formulations with the short horizon length. However, the OL-DRTO does not account for the closed-loop controller effect on the process. figure 5.14 shows the simulation result for the OL-DRTO-MPC formulation. The input set point changes in Figure 5.14 shows that the OL-DRTO layer requests maximum available U_1 action and in-turn reduces the contribution of the expensive input U_2. The U_1 input changes in this figure shows that the OL-DRTO layer could not accomplish a similar compromise which is observed in the CL-DRTO-MPC simulation result. Thus, the economic optimization layer could not leverage the economic improvement by the supervision of the detuned MPC control layer. A more detailed performance comparison of the OL- and CL-DRTO-MPC has been carried out in Jamaludin and Swartz [2016] and in the previous section of the current research.

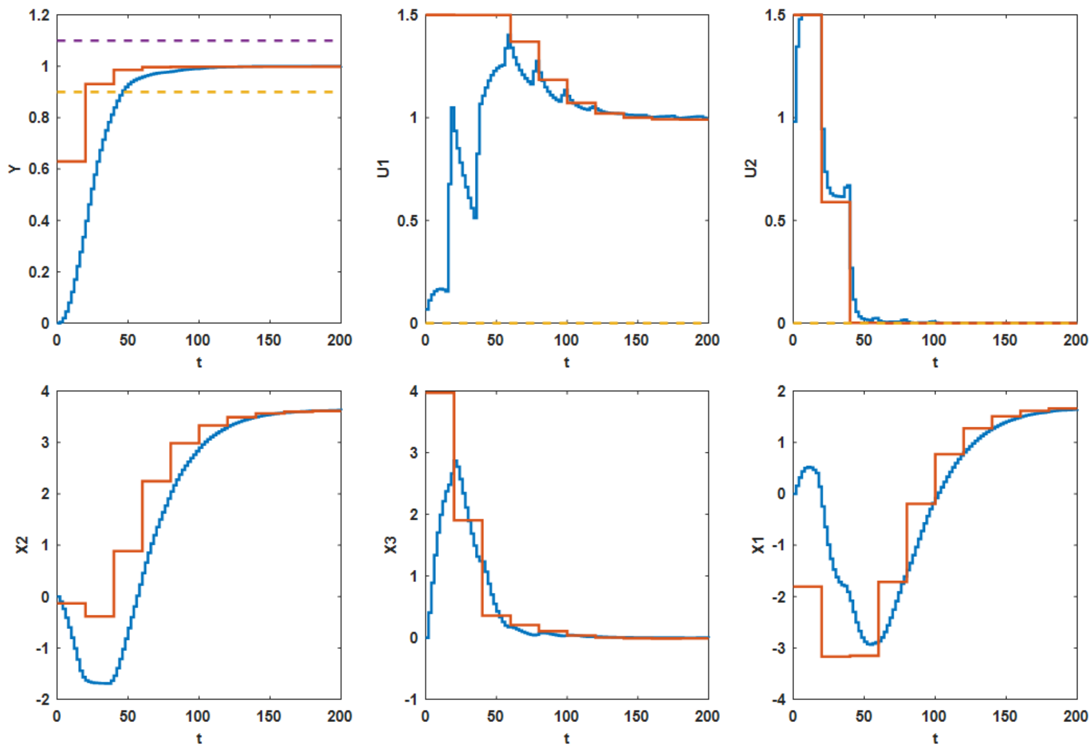

Figure 5.14: Open-loop DRTO results for $N = 30$.

Results of table 5.2 shows that the CL-DRTO-MPC has the smallest OCE which means it has the capability to skillfully distribute the smallest control effort over the horizon length and result in relatively high economic return for a reasonably efficient ART. The results of table 5.2 shows that the EMPC formulations with the longer horizon would achieve a slightly higher economic performance. However, as mentioned by Ellis and Christofides [2014a], EMPC with a large horizon length and update time equal to that of the MPC control layer in the dual-layer method results in a large NLP problem size. Therefore, the EMPC with a long horizon may not be appropriate for online application. Thus, EMPC with the long horizons of $N = 30$, and 50 are solved for the larger update time $T_e = 10s$ and the same economic horizon length. EMPC applications with a large update time are susceptible to process model mismatch and unknown disturbance effects (Ochoa *et al.* [2010]).

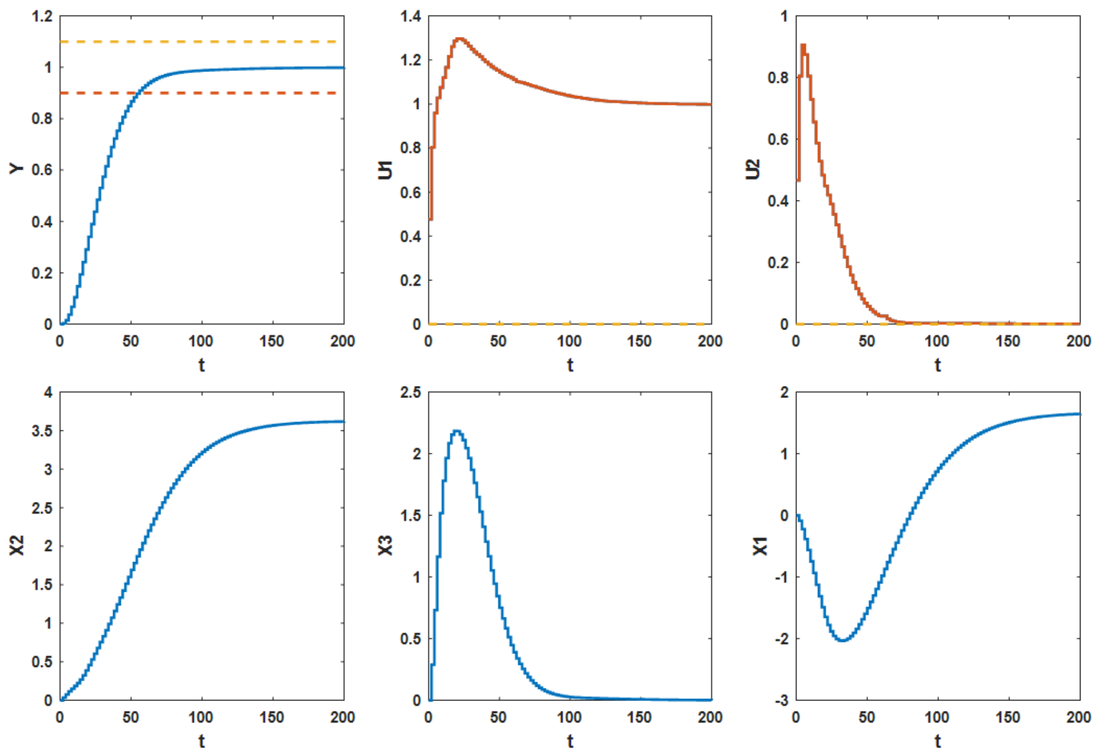

Figure 5.15: EMPC results for $N = 3$.

5.7 Recycle effects on the linear systems

As explained in the process description section for the overall input-output behavior of a simple linear recycle system in the form of equation 5.2, an increase in a positive value of the recycle gain K_R and/ or the recycle time constant τ_R increases the overall input-output gain and time constant. In this study, it is assumed that the recycle time constant is a small fixed parameter. Therefore, the overall process gain and the overall time constant would change due to a change in the recycle gain. In the current section, the efficient length of the economic optimization horizon is investigated for following two cases:

1. The process gain and the average time constant of the first subsystem, which is in the form of equation 5.2, are higher than the base case problem of equation 5.1.

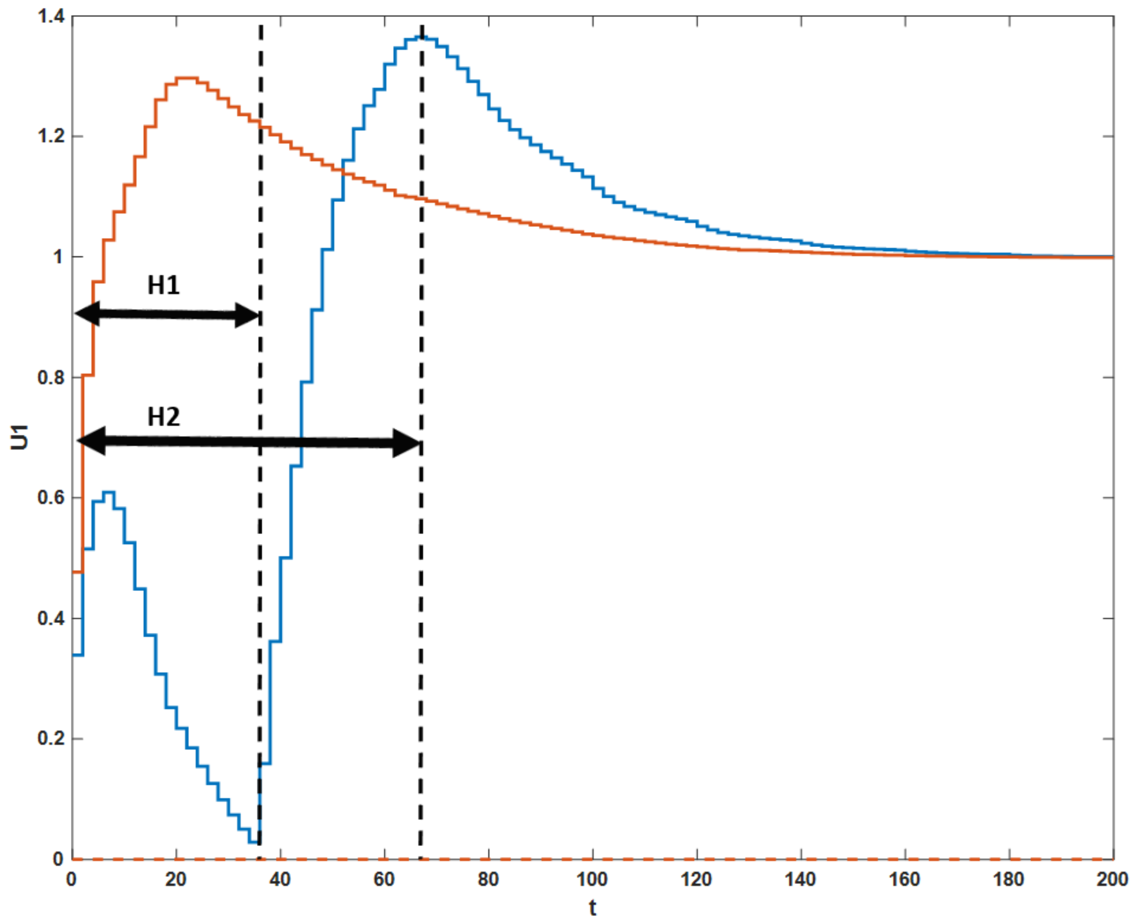

Figure 5.16: Sufficient horizon length for the control input resource saving maneuver of U_1. The input U_1 of the EMPC with a small horizon (——), and U_1 of the CL-DRTO with a large horizon (——).

2. The process gain and the average time constant of the first subsystem, which is in the form of equation 5.2, are lower than the base case problem of equation 5.1.

Simulation results of the CL-DRTO-MPC application for this two cases are shown in figures 5.17 and 5.18. A U_1 input change pattern is visible in figure 5.17 which is similar to the U_1 input maneuver of the CL-DRTO-MPC for the base case problem. The qualitative differences are the CL-DRTO tendency to use more U_2 in comparison to the base case scenario. This behavior is because of the slower U_1 input-output response comparing to the base case problem. The slow U_1 response could not settle down earlier than the end of simulation time. The slower time-scale of the U_1 input-output response suggests that a larger economic optimization horizon might be needed to recover more economic performance. The EMPC economic performance result increases from $\Phi_{eco} = 7347.0$ to 7675.3\$ by increasing the horizon length from $N = 30$ to 50. This means that the sufficient economic horizon which is $N = 30$ for the base case problem must be further increased to $N = 50$ for the EMPC formulation which causes a more intensive computational burden comparing to the base case problem. This result highlights the fact that the EMPC implementation with the update time equal to that of the MPC in the two-layer structures may not be applicable.

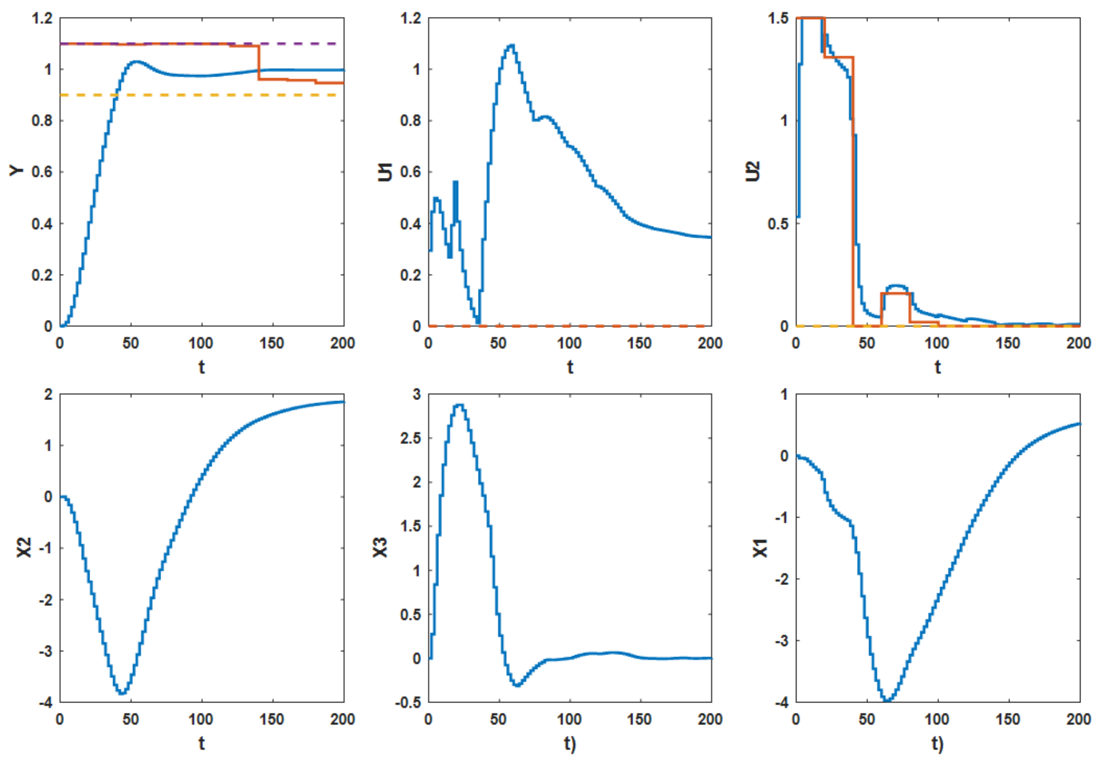

Figure 5.17: Closed-loop DRTO results with $N = 50$ for the recycle effect of case 1 (Overall gain $K_1 = 3$, and the time constants are 200 and 15 in subsystem 1).

The simulation results of figure 5.18 for the CL-DRTO-MPC implementation shows that for the smaller gain and the faster input-output response the economic optimizer highly relies on

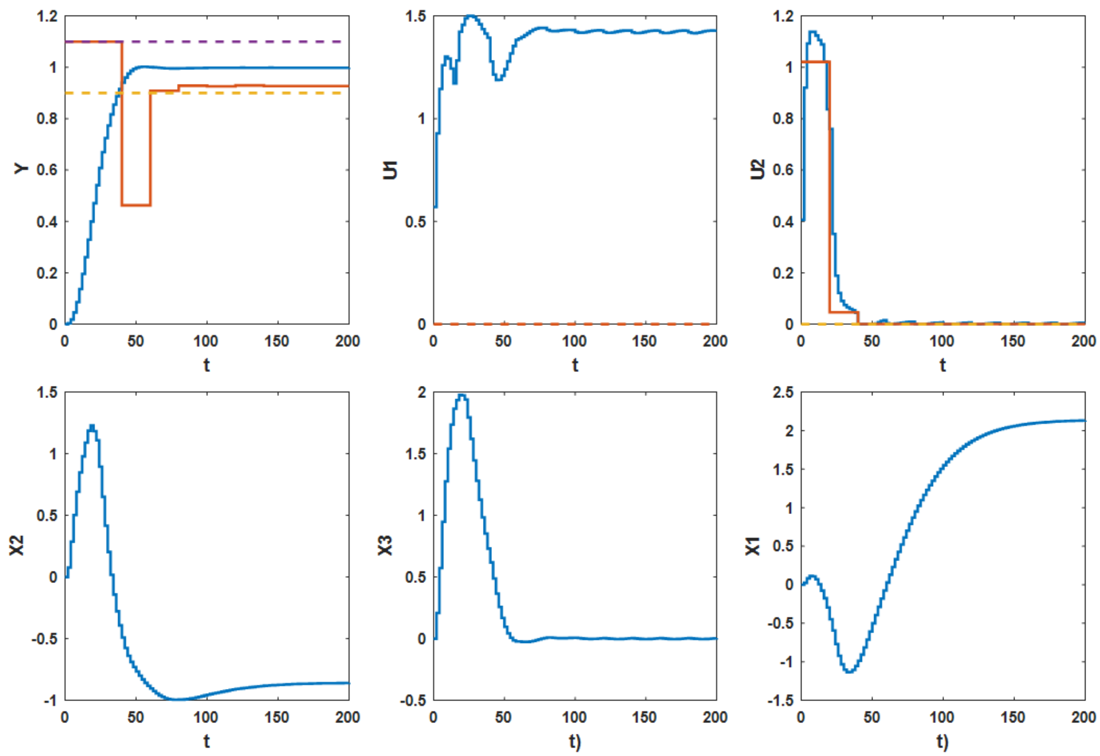

Figure 5.18: Closed-loop DRTO results with $N = 50$ for the recycle effect of case 2 (Overall gain $K_1 = 0.7$, and the time constants are 25 and 15 in subsystem 1).

the U_1 input adjustment to improve the economic performance. This behavior is expected because the first input is cheaper than U_2, and its input-output response is nearly as fast as that of the second input. After the initial input moves, there is only a rapid U_1 input change for a short interval of one DRTO update time to back-off the output from the upper bound quality constraint. As there is no considerable control input move other than the initial input changes for a large horizon of $N = 30$, no economic performance improvement would be imagined for the larger economic optimization horizon and $\Phi_{eco} = 7803.67\$$.

5.7.1 Chapter summary

In this chapter a systematic performance comparison of the single-layer EMPC, the open-loop and the closed-loop two-layer DRTO-MPC formulation is conducted for a process output dynamic transition application of a MISO linear case-study problem. The sequential approach is selected for the implementation of the economic optimization problem. In the first step the simulation results are validated using the simulation results of the simultaneous solution strategy. Then, the MPC prediction horizon effect on the economic performance and the stability of the dual-layer method is analyzed. The results suggest the use of a sufficiently long MPC horizon for stability and robustness.

The MPC prediction horizon analysis is followed by the investigation of the EMPC horizon length effect on the economic performance of the system. This result demonstrates the necessity of using a significantly large economic optimization horizon to recover more economic improvement. The necessity of a long horizon length forms a basis for the reasoning of the next step that compares the performance of the selected EMPC and DRTO formulations and shows the two-layer methods could economically outperform the single-layer method with a smaller economic optimization horizon. This desired economic performance is achieved for the computationally advantageous problem size and a slightly lower control effort.

Finally, the changes in the efficient economic horizon length is explored for the two different recycle effects. These effects are condensed in the form of the simultaneous changes in the time constant and the input-output gain for the first subsystem of the case study problem. It is shown that the two-layer formulation could be more beneficial for the systems with a slower recycle time constant and a higher recycle gain.

Chapter 6

Conclusions and Recommendations

The main contributions including the key comparison findings of the single- and dual-layer methods and a discussion on some of the important features for the proposed sequential implementation approach of the rigorous CL-DRTO formulation are summarized and the opportunities for future research work are recommended.

6.1 Conclusions

The first contributions of this thesis is that a systematic performance comparison for the single-layer EMPC and dual-layer DRTO-MPC architectures is conducted for the dynamic transition problem and a variety of the short-term and sustained unknown process disturbances. The unique aspects of this comparison study that could distinguish it from the existing literature on the performance comparison of the existing EMPC and DRTO approaches are: 1-consideration of multiple performance comparison criteria and 2-inclusion of both open-loop and closed-loop variants of the dual-layer formulation.

The key results of this comparison are that the single-layer method may not be a wise choice in the cases where the economic performance of the dual-layer methods are slightly less than that of the EMPC for an equal length of the economic optimization horizon and

1- the computational cost is significantly higher than that of the two-layer method even for the EMPC horizon length smaller than that of the dual-layer method and/ or 2- the slow time scale of the external disturbance or the process dynamics strongly affects the process economic performance. For instance, in the second case study problem, process output changes in response to the first input are slower than that of the second input. However, the first input resource is cheaper than the second input. Thus, the slower input to output response eventually should be considered for the higher economic performance. In this case, it is shown that a large economic optimization horizon is necessary to capture the slower input to output dynamic effects. We showed that a larger economic horizon length is necessary for a higher gain and slower output response of the cheaper input. The increase in the horizon length results in a bigger size NLP for the EMPC comparing to the NLP problem size in the dual-layer methods. This means the application of the EMPC, with the same MPC update time of the dual-layer methods could be computationally expensive. A recycle effect could increase the input to output gain and result in slow dynamics. A possible solution could be the use of larger economic update time in the EMPC formulation to reduce the NLP problem size. However, an inherent response delay to the unknown changes, arising from a slower EMPC update time for the first case study problem could cause a higher constraint violation (COCV). It is also shown for the transition problem in the second case study that an insufficient EMPC horizon length could cause quality grade constraint violation. As another example, for the first case-study problem in the presence of the sustained disturbance scenario, there is no need for the higher frequency of the economic update and the MPC formulation provides a satisfactory regulation function. It is also shown that the economic improvement in the presence of the sustained disturbance could be higher than a short-term disturbance with an equal unknown pulse magnitude.

Unlike the case of the sustained disturbance effect, the EMPC with a smaller update time is preferable when the short-term disturbance with a large magnitude alters the process more frequently and causes unacceptable COCV. It is shown in the first case study problem that the linear model in the MPC layer of the OL- and CL-DRTO formulation could not provide an accurate output prediction in the presence of the large magnitude disturbance while the EMPC formulation could overcome this issue due to the use of a nonlinear process model.

It is also shown that for the product grade transition the CL-DRTO-MPC formulation could result in a higher economic performance and less overall control effort comparing to that of the open-loop formulation at a cost of higher computation times.

In this study, a sequential optimization framework is chosen to avoid a large optimization problem size in the single-layer and two-layer approaches. The CL-DRTO-MPC formulation was originally developed based on the simultaneous solution approach. Therefore, a sequential implementation approach is proposed for the CL-DRTO-MPC formulation. Unlike the simultaneous implementation approach, there are no complementarity constraints in the resulting NLP problem. Thus, it does not require MPCC problem reformulation and parameter tuning for the complementarity constraint handling in a standard NLP formulation. Also, the implementation of the sequential method is easier than that of the simultaneous CL-DRTO method. However, the sequential approach has a potential drawback due to derivative discontinuities. In this study, we showed that the same solution of the simultaneous method could be achieved using the sequential approach.

6.2 Recommendations for Further Work

In the conclusion of this study, the computational cost and constraint violation are introduced as important factors which could be considered together with the economic performance to determine which one of the single- and dual-layer formulations is preferable for a process system. The EMPC formulation with a large horizon and the rigorous CL-DRTO-MPC formulations solution times could be very high and inappropriate for the real-time applications. Also, these methods may result in unacceptable constraint violations especially in the presence of the unknown disturbances and model parameter uncertainty. Therefore, there is a need to upgrade computational resources, to develop proper online optimization techniques, and to reformulate the online economic optimization problem to overcome the computational delay limitation. Therefore, following avenues could be explored in future research:

1. A method of advanced-step NMPC has been developed by Zavala and Biegler [2009a] to reduce the computational time of the dynamic optimization problems. In this method, the NLP optimization of the next NMPC step is solved using the output prediction of the process model in the background of the process operation and before the start of next NMPC update. Then, the NLP solution is updated in the next update time using the measured output and the sensitivity information of the NLP problem. The possibility of using this idea for the real-time solution of the NLP for each EMPC and/ or DRTO step could be explored.

2. The stochastic optimization methods (e.g., Min-max MPC, multi-stage NMPC) could be included in the DRTO formulation to reduce constraint violation in the presence of the unknown disturbance scenarios and model uncertainties. Lucia *et al.* [2013] applied a multi-stage MPC formulation for the control of a semi-batch polymerization reactor under uncertainty. Following this successful application of the multi-stage MPC formulation to handle the process model parameter uncertainty, they later incorporated this robust MPC technique in an EMPC formulation (Lucia *et al.* [2014]). In this method, an uncertainty horizon tree is considered which should be obtained using process knowledge and/ or statistical methods. We believe that the incorporation of this technique may potentially mitigate the constraint violation effects due to the use of a linear model in the MPC layer of the dual-layer methods.

3. As mentioned in chapter 3, the sequential approach has a potential drawback due to derivative discontinuities. However, for the second case study problem, it is shown that the same solution of the simultaneous method could be achieved using the sequential approach. Possible derivative discontinuity effects should be shown in a case study problem. This analysis could be useful to understand the discontinuity issue and to identify the conditions under which the problem converges to an acceptable solution.

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