Optimal Operation of Multiproduct Batch Plants

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Zusammenfassung in deutscher Sprache

Mehrprodukt-Batch-Anlagen (MBAn) sind für die sequenzielle Herstellung von kleinen Mengen vieler verschiedener Produkte geeignet. Diese Anlagen werden gewöhnlich dafür genutzt, hochwertige Produkte, wie Feinchemikalien, Pharmazeutika usw. herzustellen. Die wichtigsten Vorteile einer MBP sind ihre inherente Flexibilität und die Möglichkeit, auf sich ändernde Marktanforderungen schnell zu reagieren. Diese Flexibilität wird dadurch erreicht, dass verschiedene Produkte sich die gleichen Komponenten teilen (z.B. Reaktoren und Filter). Es gibt beispielsweise MBAn, in denen sogar hunderte verschieden Produkte in der gleichen Einheit hergestellt werden. Aus diesem Grund wird eine geeignete Regelung dieser Anlagen benötigt, so dass die verfügbaren Ressourcen effizient genutzt werden, um einen maximalen Profit zu erzielen. Das Optimierungsproblem für MBAn kann wie folgt formuliert werden: Gegeben seien das dynamische Modell f"ur jeden Prozess, die verfügbaren Komponenten (Reaktoren, Filter usw.) mit ihren Kapazitäten und Speicherstrategien (keine Wartezeiten, unbegrenzte Zwischenspeicher usw.) sowie die verfügbare Speicherkapazitäten für alle Materialien. Das Problem ist die Festlegung einer optimalen Sequenz von Aufgaben, die in jeder Komponente stattfinden, die Materialmenge, die verwendet wird, und die Zeitdauer jeder Aufgabe in jeder Komponente, so dass die gewünschten Ziele (Maximierung des Profits, Minimierung der Produktionsdauer etc.) erreicht werden und gleichzeitig die Marktanforderungen in einem gegeben Zeithorizont erfüllt werden.

Das oben beschriebene Optimierungsproblem für MBAn ist eine sehr komplexe hybride Optimierungsaufgabe, da sie sowohl diskrete als auch kontinuierliche Stelleingriffe beinhaltet. In der Praxis werden Ansätze benutzt, die auf standardisierten Rezepten für Produktionsabläufe basieren, wobei zunächst die Rezepte empirisch oder durch Optimierung eines einzelnen Batches (unter Nutzung der dynamischen Modelle jedes Prozesses) standardisiert werden und anschließend das Optimierungsproblem basierend auf diesen Standardrezepten formuliert wird. Allerdings führt die Standardisierung von Rezepten zur Reduzierung von Freiheitsgraden des Systems und somit können die Lösungen, die durch dieses Ansatz gewonnen werden, suboptimal sein, da sie durch vorgefertigte Produktionsrezepte eingeschränkt werden. Ein anderer Hauptnachteil dieser rezeptbasierten Ansätze besteht darin, dass es keine standardisierten Richtlinien gibt, welche festlegen wie ein geeignetes Standardrezept aussehen sollte. Für denselben Prozess kann es verschiedene widersprüchliche Rezepte geben und es gibt kein Verfahren zu entscheiden, welches dieser Rezepte das geeignetste zur Formulierung des gesamten Optimierungsproblems ist.

Der "ideale Ansatz" zur Optimierung von MBAn ist, das dynamische Modell jedes Prozesses direkt in die Formulierung des Problems zu integrieren anstatt auf standardisierte Produktionsrezepte zurückzugreifen. Dies erhält die Freiheitsgrade des Systems (die ansonsten wegen der standardisierten Produktionsrezepte wegfallen würden) und somit liefert dieser Ansatz potenziell Lösungen, die besser sind wie die mit dem rezeptbasierten Ansätzen gewonnenen Lösungen. Die direkte Einbindung der dynamischen Modelle, welche meist differenziell-algebraische Gleichungen (DAEs) sind, ergibt ein "sehr umfangreiches" nichtlineares mixed-integer dynamisches Optimierungsproblem (MIDO). Die kombinatorische Komplexität von MBAen und das Fehlen von Standardlösungsmethoden für MIDO-Probleme macht diesen Ansatz rechentechnisch für die meisten reale Probleme unlösbar. Deshalb sind neue Ansätze notwendig, die bessere Lösungen liefern als die existierenden rezeptbasierten Ansätze und gleichzeitig rechentechnisch lösbar für reale Probleme sind.

Ein verbesserter Ansatz zur Optimierung von MBAn, der durch die Einführung einer geeigneten Lösungsstruktur die Anzahl der Freiheitsgrade zwar reduziert, sich aber gleichzeitig nur wenig auf das Kostenfunktional auswirkt, wird in dieser Arbeit vorgestellt. Die Effektivität dieses Ansatzes wird mit Hilfe von verschiedenen Anwendungsbeispielen veranschaulicht.

Abstract

Multiproduct batch plants (MBPs), also known as specialty plants, are capable of sequentially producing small amounts of a large number of different products. These plants are commonly used for producing very high value products such as fine chemicals, pharmaceuticals etc. The most important features that make MBPs particularly attractive are their inherent flexibility and the ability to respond quickly to the changing market demands. Owing this inherent flexibility, in MBPs several products share the same units (for e.g., reactors, purificators etc.). There are examples of MBPs where even hundreds of products are processed in the same unit. This mandates the need for proper control of these plants so as to utilize the available resources efficiently and achieve maximum profit. The optimal control problem for the MBPs can be formally stated as: given the dynamic model for each of the processes, available units (reactors, purificators etc.) along with their capacity limits, the storage policy (zero-wait, unlimited intermediate storage etc.) to be followed and available storage capacity for each of the materials, determine the optimal sequence of tasks taking place on each unit, the amount of material being processed and the duration of each task on each unit, so as to achieve the desired objective (maximization of profit, minimization of make-span etc.) while satisfying the market demands within the given time horizon.

The above mentioned optimal control problem of MBPs is a highly non-trivial hybrid control problem as it involves both discrete and continuous decisions. In practice, approaches based on standard production recipes are used, where first the recipes are standardized either empirically or via single batch optimization (using the dynamic models of each of the processes) and then the control problem is formulated on the basis of these standardized recipes. However, standardization of recipes removes degrees of freedom from the system and hence the solutions obtained with this approach can be suboptimal as they are confined to pre-determined standard production recipes. Another major disadvantage of these standard recipe based approaches arises from the fact that there are no standard

guidelines available for deciding what a suitable standard recipe should be. For the same process there can be several conflicting recipes and there is no way to decide which one of these recipes would be the most suitable for the overall control problem formulation.

The “ideal approach” for the optimal control of MBPs is to include the dynamic model of each of the processes directly into the control problem formulation instead of standardized production recipes. This restores the additional degrees of freedom of the system (which were otherwise removed due to the standardization of the production recipe) and hence this approach potentially yields solutions that are usually much better or at least as good as that obtained with the standard recipe based approaches. However, direct inclusion of the dynamic models, which are usually differential algebraic equations (DAEs), results in a “large” nonlinear mixed-integer dynamic optimization (MIDO) problem. The combinatorial complexity of MBPs and lack of standard solution methods for MIDO problems render this approach computationally intractable for real world problems. This mandates the need for novel approaches which can yield better solutions than the existing standard recipe based approaches and at the same time are computationally tractable for real world problems.

An improved approach for the optimal control of MBPs, which, by imposing a suitable solution structure reduces the degrees of freedom of the system while only slightly affecting the achievable performance, is proposed in this work. This approach helps to recover the solution theoretically obtainable by the “ideal approach” more closely than that by the standard recipe approach while keeping a lid on the complexity. The effectiveness of this approach is illustrated with the help of several application examples.

Nomenclature

General nomenclature for all the chapters

Indices

i	index relating to tasks
j	index relating to units
n	index relating to event points representing the beginning of a task or unit utilization
s	index relating to states

Sets

I	set of tasks
I_j	set of tasks which can be performed in unit j
I_s	set of tasks processing (producing or consuming) state s
J	set of units
J_i	set of units which are suitable for performing task i
N	set of event points within the time horizon
S	set of all involved states s

Parameters

C_{ij}^{min}	minimum capacity for carrying out task i on unit j
C_{ij}^{max}	maximum capacity of unit j while executing task i
md_s	market demand for state s to be satisfied at the end of the time horizon
P_{si}^{p}	proportion of state s produced from task i
P_{si}^{c}	proportion of state s consumed by task i
M	time horizon or the total makespan

st_s^{max}	maximum storage capacity available for state s
H	a large scalar, should be greater than the time horizon under consideration
$T_{jii'}^{cl}$	cleaning time required between tasks i and i' at unit j

Variables

$te(i,n)$	$te(i,n) \in \{0,1\}$, where $\{te(i,n) = 1\}$ signifies the beginning of task i at event point n
$ue(j,n)$	$ue(j,n) \in \{0,1\}$, where $\{ue(i,n) = 1\}$ signifies the beginning of utilization of unit j at event point n
$vol(i,j,n)$	amount of material undergoing task i in unit j at event point n, $i \in I_j$ referred simply as vol (*i.e.*, without the indices) when discussing an individual task on an individual unit
$d(s,n)$	amount of state s going to the market at event point n
$st(s,n)$	amount of state s at event point n
$T^s(i,j,n)$	starting time of task i in unit j at event point n, $i \in I_j$
$T^f(i,j,n)$	finishing time of task i in unit j at event point n, $i \in I_j$
$dur(i,j,n)$	duration of task i in unit j at event point n, $i \in I_j$ referred simply as dur (*i.e.*, without the indices) when discussing an individual task on an individual unit
$dur_0(i,j,n)$	minimum processing duration for task i in unit j at event point n, $i \in I_j$ referred simply as dur_0 (*i.e.*, without the indices) when discussing an individual task on an individual unit
$\delta(i,j,n)$	absolute minimum of all "residuals" that are less than zero for task i in unit j at event point n, $i \in I_j$
$Qr(i,j,n)$	resources (e.g., energy, etc.) required for task i in unit j at event point n, $i \in I_j$ referred simply as Qr (*i.e.*, without the indices) when discussing an individual task on an individual unit
$z_{ijn}(t)$	vector of state variables for task i in unit j at time t, where t starts at $T^s(i,j,n)$ referred simply as $z(t)$ (*i.e.*, without the subscripts) when discussing an individual task on an individual unit
$u_{ijn}(t)$	control variables for task i in unit j at time t, where t starts at $T^s(i,j,n)$ referred simply as $Qr(t)$ (*i.e.*, without the subscripts) when discussing an individual task on an individual unit

Chapter-specific nomenclature

Chapter2

$c_a(t)$	concentration of reactant A at time t $[kg/m^3]$
$c_b(t)$	concentration of product B at time t $[kg/m^3]$
$v(t)$	kinetic rate constant (transformed control variable) $[hour^{-1}]$
α	kinetic parameter in example 1
β	kinetic parameter in example 1 $[hour^{\alpha-1}]$
α_k	kinetic parameter for reaction k in example 2 $[hour^{\beta_k-1}]$
β_k	kinetic parameter for reaction k in example 2
$X_{A_k}(t)$	total moles of reactant A in reaction k at time t $[kmoles]$
C_{A_k}	concentration of reactant A in the feed for reaction k $[kmoles/m^3]$
$X_{P_k}(t)$	total moles of reactant P in reaction k at time t $[kmoles]$
$X_{W_k}(t)$	total moles of reactant W in reaction k at time t $[kmoles]$
$u_k(t)$	kinetic rate constant (transformed control variable) $[hour^{-1}]$
$F_{A_k}(t)$	feed flow rate of reactant A in reaction k at time t $[m^3/hour]$
$V_k(t)$	volume of the reactor mixture during reaction k at time t $[m^3]$
vol_k	batch size for reaction k $[m^3]$
dur_k	duration of reaction k $[hours]$
Qr_k	energy resource required for reaction k

Chapter4

A_{i_r}	inner surface area of reactor r, where $r \in \{1, 2\}$ $[m^2]$
A_{o_r}	outer surface area of reactor $r[m^2]$
$C_{i_x}(t)$	concentration of component i in reaction x at time t $[kmol/m^3]$
C_{p_x}	specific heat of the reactant in reaction x $[J/kg\ K]$
C_{pm}	specific heat of the reactor/purificator metal $[J/kg\ K]$
C_{pJ}	specific heat of the coolant/hot water $[J/kg\ K]$
E_{1_x}	activation energy 1 for reaction x $[J/kmol]$
E_{2_x}	activation energy 2 for reaction x $[J/kmol]$
$F_{J_x}(t)$	coolant flow rate at time t for reaction x $[m^3/h]$
ΔH_{1_x}	enthalpy of reaction 1 for reaction x $[J/kmol]$
ΔH_{2_x}	enthalpy of reaction 2 for reaction x $[J/kmol]$

k_{1_x}	reaction rate constant 1 for reaction x
k_{2_x}	reaction rate constant 2 for reaction x
k_{10_x}	frequency factor 1 for reaction x $[hour^{-1}]$
k_{20_x}	frequency factor 2 for reaction x $[hour^{-1}]$
Q_{r_x}	heat generated during reaction x
Q_{J_x}	amount of heat transferred to the coolant in reaction x
Q_{m_x}	amount of heat transferred to the reactor metal in reaction x
R	universal gas constant $[J/kmol\ K]$
$T_x(t)$	temperature of the reaction mixture at time t in reaction x $[K]$
$T_{J_x}(t)$	temperature of coolant at time t in reaction x $[K]$
T_{J0}	inlet temperature of coolant $[K]$
$T_{m_x}(t)$	temperature of the reactor metal at time t in reaction x $[K]$
U_i	inside heat transfer coefficient of the reactor/purificator metal $[J/h\ K\ m^2]$
U_o	outside heat transfer coefficient of the reactor/purificator metal $[J/h\ K\ m^2]$
V_x	volume of the reactor contents in reaction x $[m^3]$
V_{J_r}	volume of the jacket of reactor r $[m^3]$
V_{m_r}	volume of the reactor metal of reactor r $[m^3]$
ρ_x	density of the reacting mixture in reaction x $[kg/m^3]$
ρ_m	density of the reactor/purificator metal $[kg/m^3]$
ρ_J	density of the coolant/hot water $[kg/m^3]$
$coolant_x$	total amount of coolant needed for reaction x $[m^3]$
T_{up_x}	upper bound on the temperature of the reacting mixture during reaction x $[K]$
T_{sat_x}	saturation temperature of the intermediate produced from reaction x $[K]$
$C_{A_x}(t)$	concentration of reactant A at time t in reaction x $[kmol/m^3]$
$C_{B_x}(t)$	concentration of product B at time t in reaction x $[kmol/m^3]$
$C_{C_x}(t)$	concentration of by-product C at time t in reaction x $[kmol/m^3]$
$C_{C_{max_x}}$	upper limit on the amount of by-product produced during reaction x $[kmol/m^3]$
$C_{B_{int_x}}$	final concentration of the desired product B in the intermediate produced from reaction x $[kmol/m^3]$
A_i	inner surface area of the purificators $[m^2]$
A_o	outer surface area of the purificators $[m^2]$
$T_{J_{xp}}(t)$	temperature of hot water at time t while purifying the intermediate produced from reaction x $[K]$
$T_{J_{in}}$	inlet temperature of hot water $[K]$
$T_{m_{xp}}(t)$	temperature of the purificator metal (wall) at time t while purifying the intermediate produced from reaction x $[K]$

$V_{xp}(t)$	volume of the purificator content at time t while purifying the intermediate produced from reaction x $[m^3]$
$V_{0_{xp}}$	initial volume of the purificator content while purifying the intermediate produced from reaction x $[m^3]$
$M_{v_{xp}}$	mass flowrate of vapor while purifying the intermediate produced from reaction x $[kg/h]$
$H_{v_{xp}}$	enthalpy of the vapor leaving the purificator while purifying the intermediate produced from reaction x
$H_{xp}(t)$	enthalpy of the intermediate produced from reaction x at time t during purification
V_J	volume of the jacket of the purificator $[m^3]$
V_m	volume of the purificator metal $[m^3]$
H_{latent_x}	latent heat of the intermediate produced from reaction x $[J/kg]$
$F_{J_{xp}}(t)$	hot water flow rate at time t while purifying the intermediate produced from reaction x $[m^3/h]$
$C_{B_{xp}}(t)$	concentration of product B at time t while purifying the intermediate produced from reaction x $[kmol/m^3]$
$C_{B_{0_{xp}}}$	initial concentration of product B while purifying the intermediate produced from reaction x, note that $C_{B_{0_{xp}}} = C_{B_{int_x}}$ $[kmol/m^3]$
$C_{B_{f_{xp}}}$	final concentration of product B while purifying the intermediate produced from reaction x $[kmol/m^3]$
$hot\ water_{xp}$	total amount of hot water needed while purifying the intermediate produced from reaction x $[m^3]$

AppendixB

Indices

l	index relating to time-points
c	index relating to control-intervals

Sets

L	set of time-points
C	set of control-intervals

Variables

$z(c,l)$	value of state variables z at time-point l within control-interval c
$u(c)$	value of control variables u within control-interval c
$step(c,l)$	spacing between time-points l and $l+1$ within control-interval c

List of Abbreviations

DAEs	Differential Algebraic Equations
DO	Dynamic Optimization
IA	Improved Approach
MBPs	Multiproduct Batch Plants
MIDO	Mixed-Integer Dynamic Optimization
MILP	Mixed-Integer Linear Programming
MINLP	Mixed-Integer Nonlinear Programming
MU	Money Unit
NLP	Nonlinear Programming Problem
ODEs	Ordinary Differential Equations
OOA	Overall Optimization Approach
SBO	Single Batch Optimization
SRA	Standard Recipe Approach
STN	State Task Network

Chapter 1

Introduction

Multi-product batch plants (MBPs), also termed as specialty plants, are capable of sequentially producing small amounts of a large number of different products. These plants are commonly used for producing very high value products (sales price usually in the range of 5 - 500 Euros/kg [38]) such as foods, fine chemicals, pharmaceuticals etc. MBPs are of particular importance in the chemical manufacturing arena as nearly 80 % of the products produced in these plants are found to be in steady and growing business [34]. The most important features that make MBPs particularly attractive are their inherent flexibility and the ability to respond quickly to the ever changing market demands [42].

An example multi-product batch plant comprising of two semi-batch reactors (R1 and R2) and three batch filters (F1, F2 and F3) is shown in Figure 1.1. Three different products (P_1, P_2 and P_3) are produced in this plant from three different raw materials (A_1, A_2 and A_3) as per the following reaction scheme:

$$\begin{gathered} A_k \longrightarrow P_k \\ A_k \longrightarrow W_k \quad ; \qquad k = 1, 2, 3 \\ A_k = \text{reactant},\ P_k = \text{product},\ W_k = \text{waste} \end{gathered}$$

All of these reactions are carried out in the presence of a large amount of solvent, which is stored in the solvent tank shown in Figure 1.1. It is assumed that for every reaction the amount of solvent contributes 90% of the given batch size. Before every reaction, the reactors are filled with the required amount of solvent and then the reactants are dosed strategically. At the end of the reactions, the intermediates from these reactors are sent to the filters, where they are split volumetrically into the solvent (90%) and the respective products (10%). The recovered solvent is sent back to the solvent tank and can be used for further reactions.

Each of these reactions and the subsequent filtrations can be carried out in any of the reactors and the filters respectively. Thus, we see that in MBPs several products share the same units (for e.g., the reactors and the filters in this case). This is true for every MBP. There are examples of MBPs, where even hundreds of different products are processed in the same unit [35].

Optimal operation of these plants is a highly non-trivial hybrid control problem as it involves both discrete and continuous decisions. The discrete decisions usually involve selection of proper sequence in which the products are to be produced and the units allocated for producing them. Whereas, the continuous decisions usually involve determination of suitable control input signals, amounts of materials to be processed at a time on a given unit and the processing durations dedicated to them.

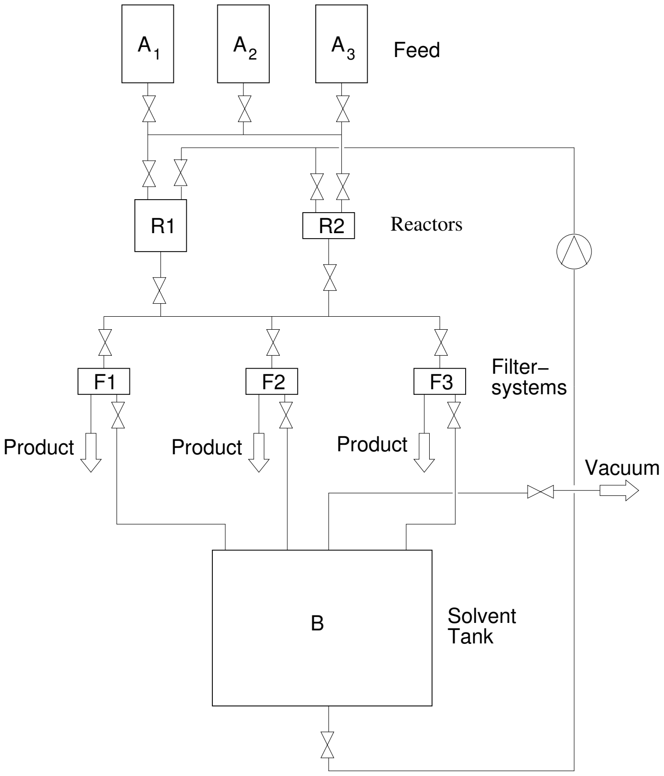

Figure 1.1: An example multi-product batch plant.

1.1 The Control Problem Statement

The control problem of the MBPs considered in this work can be formally stated as follows:
Given the dynamic models for each of the processes ($i.e.$, the stoichiometric balances, rate equations, safety constraints etc.), available units (reactors, purificators etc.) along with their capacity limits, the storage policy (zero-wait, unlimited intermediate storage etc.) to be followed and available storage capacity for each of the materials, determine the optimal sequence of tasks taking place on each unit, the amount of material being processed and the duration of each task on each unit, so as to achieve the desired objective (maximization of profit, minimization of makespan etc.) while satisfying the market demands within the time horizon.

This boils down to the determination of open loop optimal control policy for the plant. Aspects of feedback control are not taken into account in this work.

1.2 General Structure of the Control Problem

The control problem formulation of the MBPs can be divided into the following two steps:

1. **Graphical representation of the process under consideration.**
   Graphical representation of the process network is very important for a better understanding of the tasks involved in the process and the interconnections between them. There are several approaches available for this in the literature. Out of which, some of the most prominent ones are the state-task network (STN) representation proposed by Kondili et al. [24], the resource-task network (RTN) representation proposed by Schilling and Pantelides [44] and the state-sequence network (SSN) proposed by Zhu and Majozi [26]. Throughout this work, the STN is used for graphically representing the processes and hence, it is discussed in detail in the following.

   The state-task network (STN) is a very powerful mean for the graphical representation of chemical processes and particularly, batch processes involving a large variety of complexities can be unambiguously represented by it. In STN, all of the materials (reactants, intermediates, final products, etc.) involved in the process are marked as ”states” and are denoted by circles. Whereas, all the processing steps (reaction, purification, etc.), which transform one or more input states to one or more output states are marked as ”tasks” and are denoted by rectangles.

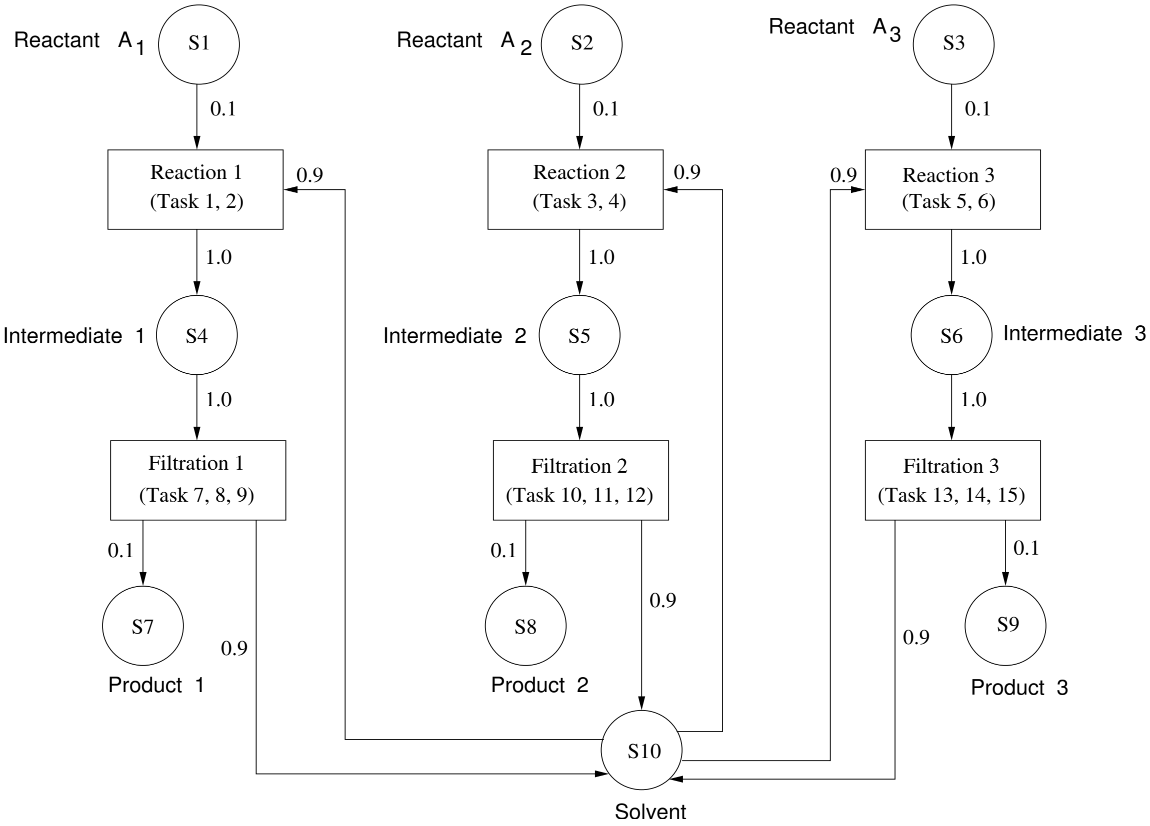

Figure 1.2: State-task-network representation of the process shown in Figure 1.1.

As an example, the STN representation for the MBP shown in Figure 1.1 is presented in Figure 1.2. Where, all the reactants (A_1, A_2 and A_3), the intermediates (intermediate 1, 2 and 3) the products(P_1, P_2 and P_3) and the solvent are denoted by states S1 - S10, respectively. The three reaction tasks and the respective filtration tasks are denoted by rectangles. The flow of materials within the process is indicated by means of arrows. An arrow pointing towards a given rectangle indicates that the connecting state is being consumed by the task represented by that rectangle, whereas, an arrow pointing away from the rectangle indicates that the connecting state is being produced by that task. The proportion of a state being produced or consumed by a connected task is indicated alongside the arrows. It needs to be mentioned that the units (reactors, filters, etc.) are never shown explicitly in the STN. For a detailed description of the STNs and their various capabilities, the reader is kindly referred to Appendix A.

2. **Control problem formulation.**

   The control problem of MBPs, considered throughout this work, is nothing but a mathematical optimization problem, where the goal is to realize a certain objective (maximization of the sales revenue, minimization of the makespan, etc.) while satisfying the various process constraints as well as the market requirements.

   Extensive research has been done in this area [24, 31, 32, 44, 18, 25, 16, 26, 8, 3, 15, 19, 20, 30, 33, 36, 37, 43, 48, 27]. and several elegant approaches have been proposed in the literature for the control problem formulation of the MBPs. Depending on their handling of the process dynamics, these approaches can be broadly classified into the following:

   - **The standard recipe approach (SRA)**

     Most of the control problem formulations proposed in the literature are based on this approach [24, 31, 32, 44, 18, 25, 16, 26, 3, 15, 19, 20, 30, 33, 36, 37, 48, 27]. A schematic representation of this approach is presented in Figure 1.3. In this approach, first a standard production recipe (e.g., processing time, control strategy etc., for different batch sizes) is obtained either empirically or via single batch optimization (SBO) using the dynamic models of the processes and then, the control problem is formulated using this standard production recipe. The control problem obtained with this approach is either a mixed-integer nonlinear programming (MINLP) problem or a mixed-integer linear programming (MILP) problem, which can be approached using conventional solvers readily available in the market. However, this approach suffers from a major drawback, which arises due to the use of standard production recipe. Standardization of recipe removes degrees of freedom from the system and hence, the solution obtained with this approach is expected to be suboptimal.

   - **The overall optimization approach (OOA)**

     This approach was first discussed by Bhatia and Biegler [8]. Figure 1.4 presents a schematic representation of this approach. In this approach, the dynamic models of the processes are directly included in the control problem formulation instead of the standard production recipe. However, direct inclusion of the dynamic models of the processes in the control problem formulation results in a mixed-integer dynamic optimization (MIDO) problem, the solution of which can be a formidable task. The present trend of approaching these infinite-dimensional MIDO problems is to transform them into finite-dimensional MINLP problems [4, 5] via suitable time discretization schemes like the standard trapezoidal rule, the orthogonal collocation on finite elements etc. However, the MINLP problems obtained by discretizing the MIDO problems in time are usually very large and hence computationally difficult or even impossible to solve for problems of practical size.

The SRA and the OOA both suffer from some serious drawbacks, as mentioned above. This mandates the need for novel approaches for the control of this important class of chemical plants, which can yield better solutions than the SRA and at the same time result in computationally tractable control problems. An improved approach, which promises to overcome the drawbacks of both the SRA and the OOA upto a large extent, is proposed

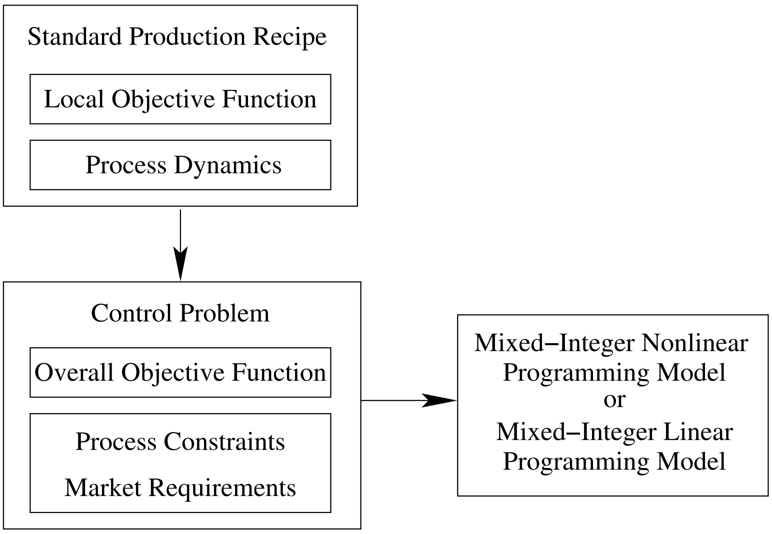

Figure 1.3: Schematic representation of the standard recipe approach (SRA).

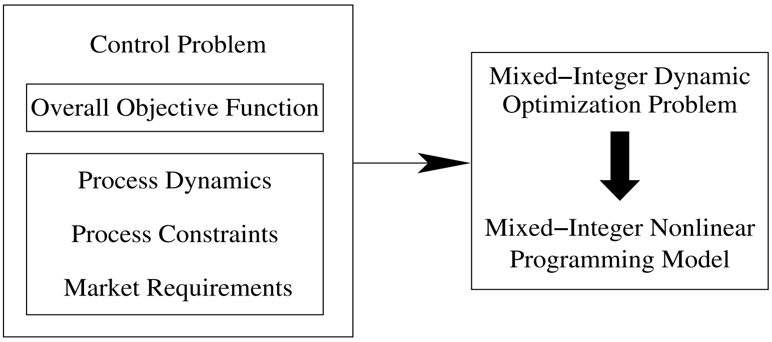

Figure 1.4: Schematic representation of the overall optimization approach (OOA).

in this thesis.

1.3 Outline

The remainder of this thesis is organized as follows. Chapter 2 presents a comparative study of the SRA and the OOA. The advantages and disadvantages of both these approaches are discussed in detail with the help of illustrative examples. Chapter 3 presents an improved approach for the control of MBPs and illustrates its effectiveness by comparing its performance to that of the SRA and the OOA for the illustrative examples. A detailed application example is presented in chapter 4. Finally, the conclusions and the directions for future research are presented in chapter 5.

Chapter 2

A Comparative Study of Different Approaches

The objective of this chapter is to present a comparative study of the SRA and the OOA. The main advantages and disadvantages of both these approaches are illustrated with the help of simple examples.

As mentioned earlier, the STN representation is used for the graphical depiction of the process. An event-point based continuous-time formulation proposed by Ierapetritou and Floudas [18, 19, 20] is adopted for the control problem formulation. The following section presents the mathematical formulation of the control problem.

2.1 Mathematical formulation of the control problem

The control problem is formulated as per the continuous time formulation proposed by Ierapetritou and Floudas [18]. The most important ingredients of the problem formulation presented in their work are reproduced here for the sake of completeness and so as to work out clearly how the process dynamics fit into this formulation. For detailed information, the reader is kindly referred to the original work of Ierapetritou and Floudas [18, 19, 20]).

In this approach, first a necessary number of *event points* ($n = 1 \ldots n_{last}$) are defined for each unit at unknown locations on the makespan. The total number of these *event points* for each unit is the same, however, they can be located differently on the makespan. The initiation of a task ($i.e.$, reaction or purification) or the beginning of an unit ($i.e.$, reactor or purificator) utilization can happen exactly at these *event points*. The other constraints for the control problem are also then formulated on the basis of these *event points*.

The following notations are used in the control problem formulation :
Indices
index i relates to tasks
index j relates to units
index n relates to event points representing the beginning of a task or unit utilization
index s relates to states

Sets
I . . . set of tasks
I_j . . . set of tasks which can be performed in unit j
I_s . . . set of tasks processing (producing or consuming) state s
J . . . set of units
J_i . . . set of units which are suitable for performing task i
N . . . set of event points within the time horizon
S . . . set of all involved states s

Parameters
C_{ij}^{min} . . . minimum capacity for carrying out task i on unit j
C_{ij}^{max} . . . maximum capacity of unit j while executing task i
md_s . . . market demand for state s to be satisfied at the end of the time horizon
P_{si}^{p} . . . proportion of state s produced from task i
P_{si}^{c} . . . proportion of state s consumed by task i
M . . . time horizon or the total makespan
st_s^{max} . . . maximum storage capacity available for state s
H . . . a large scalar, should be greater than the time horizon under consideration
$T_{jii'}^{cl}$ . . . cleaning time required between tasks i and i' at unit j

Variables
$te(i,n) \in \{0,1\}$, where $\{te(i,n) = 1\}$ signifies the beginning of task i at event point n
$ue(j,n) \in \{0,1\}$, where $\{ue(i,n) = 1\}$ signifies the beginning of utilization of unit j at event point n
$vol(i,j,n)$ . . . amount of material undergoing task i in unit j at event point n, $i \in I_j$
$d(s,n)$ . . . amount of state s going to the market at event point n

$st(s,n)$ ... amount of state s at event point n
$T^s(i,j,n)$ ... starting time of task i in unit j at event point n, $i \in I_j$
$T^f(i,j,n)$ ... finishing time of task i in unit j at event point n, $i \in I_j$
$dur(i,j,n)$ ... duration of task i in unit j at event point n, $i \in I_j$
$Qr(i,j,n)$ ... resources (e.g., energy, etc.) required for task i in unit j at event point n, $i \in I_j$
$z_{ijn}(t)$ ... vector of state variables for task i in unit j at time t, where t starts at $T^s(i,j,n)$
$u_{ijn}(t)$ ... control variables for task i in unit j at time t, where t starts at $T^s(i,j,n)$

Based on this notation the control problem involves the following constraints in general :
Allocation Constraints

$$\sum_{i \in I_j} te(i,n) = ue(j,n), \quad \forall j \in J,\ n \in N \tag{2.1}$$

where, addition is defined in the sense of standard integer addition.
These constraints express that at each unit j and at an event point n not more than one of the tasks that can be performed on this unit, *i.e.*, $i \in I_j$, should take place.

Capacity Constraints

$$C_{ij}^{min} \cdot te(i,n) \le vol(i,j,n) \le C_{ij}^{max} \cdot te(i,n), \quad \forall i \in I,\ j \in J_i,\ n \in N \tag{2.2}$$

These constraints impose upper and lower bounds on the amount of material undergoing task i in unit j at event point n.

Material Balances

$$\begin{aligned} st(s,n) = st(s,n-1) - d(s,n) &+ \sum_{i \in I_s} P_{si}^{p} \sum_{j \in J_i} vol(i,j,n-1) \\ &+ \sum_{i \in I_s} P_{si}^{c} \sum_{j \in J_i} vol(i,j,n), \quad \forall s \in S,\ n \in N \end{aligned} \tag{2.3}$$

where $P_{si}^c \le 0$ and $P_{si}^p \ge 0$. As per these constraints, the amount of state s at event point n is equal to that at event point $n-1$ adjusted by any amounts produced or consumed between the event points n and $n-1$ and the amount required by the market at event point n within the time horizon. Note that, at the first event point, *i.e.*, $n = 1$,

$st(s, n-1)$ corresponds to the initial amount of state s.

Storage Constraints

$$st(s,n) \leq st_s^{max}, \quad \forall s \in S,\ n \in N \tag{2.4}$$

These constraints represent the maximum available storage capacity for each state s at event point n.

Demand Constraints

$$\sum_{n \in N} d(s,n) \geq md_s, \quad \forall s \in S \tag{2.5}$$

These constraints impose a lower bound on the amount of product to be produced so as to satisfy the market demand.

Duration Constraints

$$T^f(i,j,n) = T^s(i,j,n) + dur(i,j,n), \quad \forall i \in I,\ j \in J_i,\ n \in N \tag{2.6}$$

These constraints represent the time duration of task i in unit j at event point n.

Sequence Constraints : Same task in the same unit

$$T^s(i,j,n+1) \geq T^f(i,j,n), \quad \forall i \in I,\ j \in J_i,\ n \in N,\ n \neq n_{last} \tag{2.7}$$

These constraints imply that task i in unit j at event point $n+1$ should start only after the end of the same task being performed in the same unit at event point n.

Sequence Constraints : Different tasks in the same unit

$$\begin{aligned} T^s(i,j,n+1) \geq T^f(i',j,n) + T^{cl}_{jii'} \cdot te(i,n+1) - H \cdot (1 - te(i',n)), \\ \forall j \in J,\ i' \in I_j,\ i \in I_j,\ i \neq i',\ n \in N,\ n \neq n_{last} \end{aligned} \tag{2.8}$$

These constraints express that if tasks i and i' are taking place in the same unit j, then they should be performed at most consecutively while satisfying cleaning requirements, if any.

Sequence Constraints : Different tasks in different units

$$T^s(i,j,n+1) \;\geq\; T^f(i',j',n) \;-\; H\cdot(1-te(i',n)),$$
$$\forall i,\; i' \,\in\, I,\; j \,\in\, J_i,\; j' \,\in\, J_{i'},\; i \,\neq\, i',\; j \,\neq\, j',\; n \,\in\, N,\; n \,\neq\, n_{last} \qquad (2.9)$$

These constraints express that if tasks i and i' are performed in different units j and j', then they should be carried out consecutively adhering to the production recipe.

Sequence constraints : Same task in different units

A task that can be performed on different units is formulated as different tasks in different units using Equation 2.9 , $i.e.$, each task in each unit is considered as a different task with the same features.

Sequence Constraints : 'Zero-wait' conditions

$$T^s(i,j,n+1) \;\leq\; T^f(i',j',n) \;+\; H\cdot(2-te(i,n+1)-te(i',n)),$$
$$\forall i,\; i' \,\in\, I,\; j \,\in\, J_i,\; j' \,\in\, J_{i'},\; n \,\in\, N,\; n \,\neq\, n_{last} \qquad (2.10)$$

Combined with Equations 2.8 and 2.9, Equation 2.10 enforces that task i in unit j at event point $n+1$ starts immediately after the end of task i' in unit j' at event point n if both of them are to be performed.

Sequence Constraints : Completion of previous tasks

$$T^s(i,j,n+1) \;\geq\; \sum_{n' \,\in\, N,\; n' \,\leq\, n} \;\; \sum_{i' \,\in\, I_j} (T^f(i',j,n') - T^s(i',j,n')),$$
$$\forall i \,\in\, I,\; j \,\in\, J_i,\; n \,\in\, N,\; n \,\neq\, n_{last} \qquad (2.11)$$

Equation 2.11 imposes a lower bound on the starting time of task i in unit j at event point $n+1$.

Time Horizon Constraints

$$T^f(i,j,n) \;\leq\; M, \quad \forall i \,\in\, I,\; j \,\in\, J_i,\; n \,\in\, N \qquad (2.12)$$

Equation 2.12 ensures that every task ends within the time horizon under consideration.

Objective Function

The objective function of the control problem represents the desired performance criteria, for example, minimization of makespan, maximization of profit via sales revenue, minimization of operation costs, etc. However, in this work, we aim at maximization of the overall profit for the processing plant over a given makespan.

Process Dynamics

$\forall i \in I,\ j \in J_i,\ n \in N$

$$\frac{dz_{ijn}(t)}{dt} = f(z_{ijn}(t),\ u_{ijn}(t)) \tag{2.13}$$

$$Qr(i,j,n) = \gamma(z_{ijn}(t),\ u_{ijn}(t)) \tag{2.14}$$

$$h(z_{ijn}(t),\ u_{ijn}(t)) = 0 \tag{2.15}$$

$$g(z_{ijn}(t),\ u_{ijn}(t)) \ \leq\ 0 \tag{2.16}$$

$$h_{ep_1}(z_{ijn}(t_{ep}),\ u_{ijn}(t_{ep})) = vol(i,j,n) \tag{2.17}$$

$$h_{ep_2}(z_{ijn}(t_{ep}),\ u_{ijn}(t_{ep})) = 0 \tag{2.18}$$

$$g_{ep}(z_{ijn}(t_{ep}),\ u_{ijn}(t_{ep})) \ \leq\ 0 \tag{2.19}$$

where, $t \in [0, dur(i,j,n)]$ and $t_{ep} \in \{0, dur(i,j,n)\}$

Equations 2.13 - 2.15 represent the process model, which is in general a system of differential algebraic equations (DAEs). However, for the sake of simplicity, only systems defined solely by ordinary differential equations (ODEs) are considered in this work. Additionally, one may have path constraints 2.16 and equality 2.17, 2.18 and/or inequality 2.19 constraints at the initial and/or final time.

Based on their treatment of the process dynamics, the control approaches are classified into the SRA and the OOA, as explained in the following :

Standard Recipe Approach (SRA)

In this approach, the process dynamics do not participate directly in the control problem formulation. Instead, they are used to obtain standard recipes and then these recipes are used to simplify the control problem, as explained in detail later.

Throughout this work, the recipes are obtained by carrying out single batch optimization (SBO) of the processes described by Equations 2.13 - 2.19 (without the indices i, j and n) using suitable optimization criterion (e.g., minimization of the operation cost etc.).

$$\min_{z(t),\ u(t),\ dur} \rho(z(t),\ u(t),\ z(dur)), \quad \forall i\ \in\ I,\ j\ \in\ J_i,\ n\ \in\ N \tag{2.20}$$

subject to

$$\frac{dz(t)}{dt} = f(z(t),\ u(t)) \tag{2.21}$$

$$Qr = \gamma(z(t),\ u(t)) \tag{2.22}$$

$$h(z(t),\ u(t)) = 0 \tag{2.23}$$

$$g(z(t),\ u(t))\ \leq\ 0 \tag{2.24}$$

$$h_{ep_1}(z(t_{ep}),\ u(t_{ep})) = vol \tag{2.25}$$

$$h_{ep_2}(z(t_{ep}),\ u(t_{ep})) = 0 \tag{2.26}$$

$$g_{ep}(z(t_{ep}),\ u(t_{ep}))\ \leq\ 0 \tag{2.27}$$

where, $t \in [0, dur]$ and $t_{ep} \in \{0, dur\}$

The SBO is carried out for different batch sizes and all tasks using suitable performance criteria, as shown in Equation 2.20. This way for every task i in unit j at event point n, the processing duration $dur(i, j, n)$ and the other resources (e.g., energy requirement etc.) needed for the process $Qr(i, j, n)$, etc. is obtained for different batch sizes $vol(i, j, n)$. Subsequently, suitable polynomial fittings ψ and ϕ are then used to get Equations 2.28

and 2.29.

$\forall i \in I,\ j \in J_i,\ n \in N$

$$dur(i,j,n) = \begin{cases} 0, & vol(i,j,n) = 0 \\ \psi(vol(i,j,n)), & vol(i,j,n) > 0 \end{cases} \tag{2.28}$$

$$Qr(i,j,n) = \begin{cases} 0, & vol(i,j,n) = 0 \\ \phi(vol(i,j,n)), & vol(i,j,n) > 0 \end{cases} \tag{2.29}$$

It should be noted that Equations 2.28 and 2.29 can be highly nonlinear or non-smooth in practical cases and are expected to have residuals associated with them. Utmost care is needed while defining these equations so as to keep these residuals as low as possible.

Then, Equations 2.28 and 2.29 are used for the control problem formulation instead of the process dynamics given by 2.13 - 2.19. The resulting control problem in this approach is either a MILP or a MINLP problem depending on whether Equations 2.28, 2.29 and the objective function are linear or nonlinear respectively.

Overall Optimization Approach (OOA)

In this approach, unlike the SRA, the process dynamics (i.e., Equations 2.13 - 2.19) are directly included in the control problem formulation. The resulting control problem obtained in this case is essentially a MIDO problem, which can be transformed into a MINLP problem by using a suitable time discretization scheme.

2.2 Illustrative examples

This section presents two illustrative examples. Both the control approaches are applied to these examples and the results are compared.

2.2.1 Example 1

A single product batch plant consisting of two processing stages, namely a batch reactor and a purification unit, as shown in Figure 2.1, is considered here. The plant is assumed to be operating under zero-wait policy, *i.e.*, the intermediate from the reactor cannot be stored and has to be consumed by the purification unit as soon as the reaction ends. A brief description of the processing stages involved is as follows :

Reactor :

The reactor in the plant is a dynamic batch reactor with the following series reaction to be carried out :

$$\text{A} \longrightarrow \text{B} \longrightarrow \text{C}\,; \qquad \text{A = reactant, B = product, C = waste}$$

The governing equations for this reactor are as follows :

$$\frac{dc_a(t)}{dt} = -v(t) \cdot c_a(t)\,; \quad c_a(t=0) \;=\; 12.8\,kg/m^3 \tag{2.30}$$

$$\frac{dc_b(t)}{dt} = v(t) \cdot c_a(t) - \beta \cdot v(t)^{\alpha} \cdot c_b(t)\,; \quad c_b(t=0) \;=\; 0.0 \tag{2.31}$$

where, α = 1.44798 ; β = 0.0246 $hour^{\alpha-1}$

$$Qr = vol \cdot \int_0^{dur} v(t) \cdot dt \tag{2.32}$$

Where, $c_a(t)$ and $c_b(t)$ represent the concentrations of reactant A and product B respectively at any instant of time t ($t \in [0,\, dur]$), while their respective rate equations are given by Equations 2.30 & 2.31. α and β are kinetic parameters. $v(t)$ is a rate constant and is considered to be the control variable. In practice, $v(t)$ can be changed by changing the temperature. The amount of energy resource Qr required for this is proportional to the integral over $v(t)$ according to Equation 2.32. vol is the volume of the reacting mixture in m^3, assumed to be constant throughout the reaction. The minimum

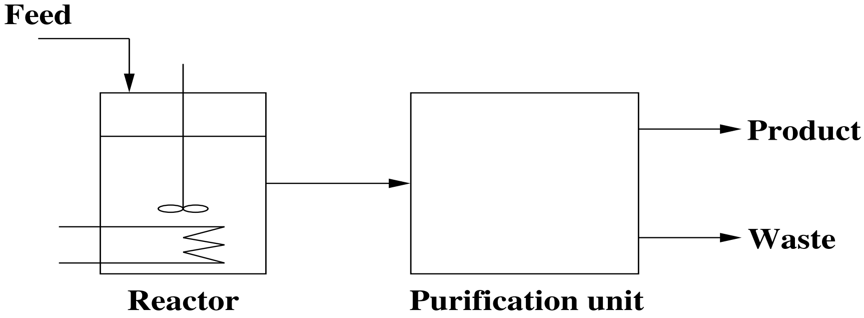

Figure 2.1: Flow sheet of the process in example 1.

volume of the reacting mixture required to start operating the reactor is assumed to be 2.0 m^3. For safe operation of the reactor, the control variable $v(t)$ is subjected to the path constraint given by Equation 2.33. Equation 2.34 represents an end constraint, which expresses the desired concentration of the product at the end of the reaction.

$$0.05647\, hour^{-1} \leq v(t) \leq 8.8885\, hour^{-1} \tag{2.33}$$

$$c_b(t = dur) = 11.52\, kg/m^3 \tag{2.34}$$

Purification Unit:

The intermediate from the reactor goes to the purification unit, where the product is separated from the waste and the unreacted reactant. The purification unit is assumed to be a separation train where the intermediate is subjected to several unit operations and is finally separated into pure product and a mixture of waste and unreacted reactant. The following simplifying assumptions are made for the operation of the purification unit :

1. The time needed for purification is directly proportional to the volume of the intermediate (from the reactor) being purified and is given as follows:
   purification duration ($hours$) = 2.0 $\cdot$ (volume of intermediate being purified (m^3))
2. The densities of reactant, product and waste are identical. Hence, the intermediate can be split volumetrically into product B and a mixture of waste C and unreacted reactant A. For example, in the above reaction the operational yield of product B is 90$\%$, which under the assumption of identical densities implies that 5 m^3 of reactant gives 4.5 m^3 of product.

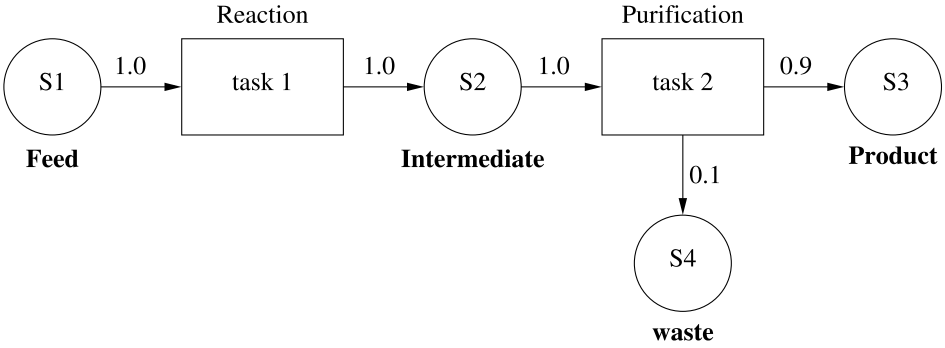

Figure 2.2: State-task-network representation of the process in example 1.

Figure 2.2 shows the state-task-network (STN) representation of the process. The basic data for the units and the states is given in Table 2.1. As an example, the following costs are assumed for running the process :

1. The running cost of the reactor is 1.2 money unit (MU) per hour.
2. The cost of resources needed for purification is 75.0 MU per m^3 of the intermediate being purified.
3. The running cost of the purification unit is 2.0 MU per hour.
4. The energy resource cost is 4.0 MU per unit Qr.

Table 2.1: Data for example 1.

Unit(j)	Capacity(m^3)	Suitability(task i)
Reactor(j=1)	5.0	Reaction(i=1)
Purificator(j=2)	5.0	Purification(i=2)
State(s)	initial amount(m^3)	price(MU per m^3)
Feed(s=1)	50.0	60.0
Intermediate(s=2)	0.0	0.0
Product(s=3)	0.0	180.0
Waste(s=4)	0.0	0.0

The control target for this example is maximization of overall profit for the plant over a fixed makespan of 10 hours, where the overall profit for the plant is defined as follows:

$$\begin{aligned} Profit &= (price\ of\ products) - (price\ of\ raw\ materials) \\ &- (running\ cost\ of\ the\ reactor) - (running\ cost\ of\ the\ purification\ unit) \\ &- (cost\ of\ resources\ needed\ for\ purification) \\ &- (energy\ resource\ cost\ of\ the\ reactor) \end{aligned}$$

Control via the SRA

The SRA for control involves determination of a standard production recipe followed by the control problem formulation on the basis of this recipe. In the present case, the recipe represents optimal heating policies for given batch sizes.

Determination of Standard Production Recipe

Reactor :
The standard production recipe for the reactor is determined via single batch optimization (SBO). For a batch reaction with fixed conversion, maximum profit can be achieved by minimization of the operation costs. So the only reasonable objective for the SBO is to minimize the total operation cost ($i.e.$, the sum of the running cost and the energy cost) of the reactor. The SBO problem (Equations 2.20 - 2.27) in this case can be written as follows:

$$minimize \quad (1.2 \cdot dur + 4.0 \cdot Qr) \tag{2.35}$$

subject to

$$Equations \;\; \text{2.30 - 2.34}$$

Hence, we have an infinite dimensional dynamic optimization problem. Appropriate discretization of the state and the control variables in time transforms this problem into a finite dimensional nonlinear programming (NLP) problem. Efficient discretization schemes based on the orthogonal collocation over finite elements [12, 13, 11, 40, 41, 45, 14, 22, 17] and moving finite elements [9] have been proposed in the literature. However, due to the simplicity of the examples chosen in this work, the standard trapezoidal rule with equidistant grids is used for discretization throughout this work. For a detailed information on the discretization technique used in this work, the reader is kindly referred to Appendix B.

The SBO is carried out for different batch sizes using 100 equidistant time points. The corresponding duration of reaction dur and energy resource requirement Qr are shown in Table 2.2. Figure 2.3 shows the reaction recipe, $i.e.$, the reaction duration and the energy required, for some of the batch sizes. Please note that the energy resource Qr required for a given batch size is given by the product of the area under the respective control profile curve ($i.e.$, $v(t)$ vs. t plot) and the batch size. Throughout this work, the NLP problems are solved using GAMS/CONOPT2 solver [1] on a Linux workstation with AMD Athlon(TM) XP 3200+ processor. The standardized equations for processing duration and energy resource requirement are obtained by fitting the optimization data shown in Table 2.2 with polynomials of appropriate order and are given by Equations

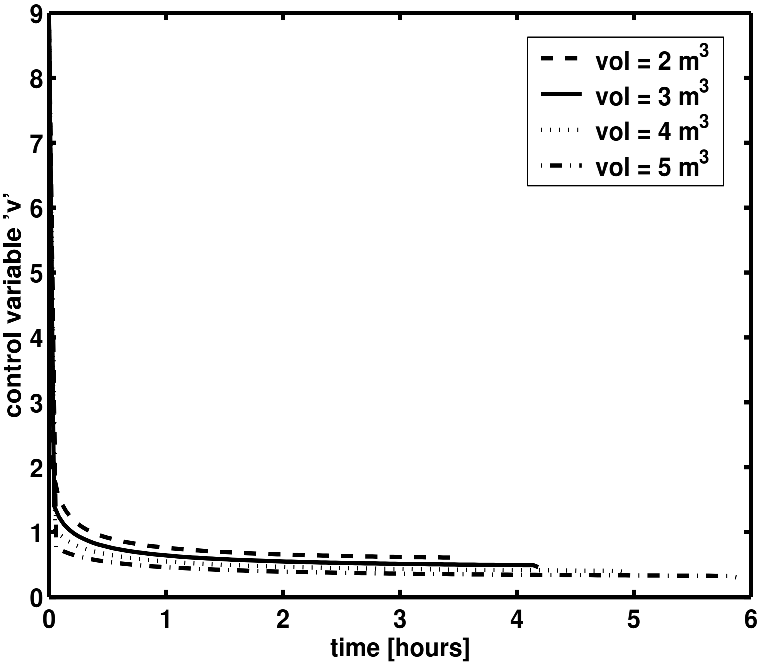

Figure 2.3: Optimal control profiles for the reaction in example 1.

2.36 and 2.37.

$$dur(1,1,n) = \begin{cases} 0, & vol(1,1,n) = 0 \\ (1.743 + 1.172 \cdot vol(1,1,n) & \\ -0.195 \cdot vol(1,1,n)^2 + 0.02518 \cdot vol(1,1,n)^3), & vol(1,1,n) > 0 \end{cases} \tag{2.36}$$

Table 2.2: Results of the SBO of the reactor in example 1.

vol(m^3)	$dur(hours)$	$Heat_f$	$Qr(m^3)$
2.0	3.5096	2.7689	5.5377
2.5	3.8423	2.7243	6.8108
3.0	4.1824	2.6871	8.0614
3.5	4.5385	2.6542	9.2897
4.0	4.9226	2.6235	10.4939
4.5	5.3546	2.5930	11.6684
5.0	5.8754	2.5601	12.8006

$$Qr(1,1,n) = \begin{cases} 0, & vol(1,1,n) = 0 \\ (0.1463 + 2.802 \cdot vol(1,1,n) & \\ -0.05396 \cdot vol(1,1,n)^2), & vol(1,1,n) > 0 \end{cases} \tag{2.37}$$

For higher accuracy, processing duration $dur(1,1,n)$ is fitted with a cubic polynomial, while for the energy requirement $Qr(1,1,n)$, quadratic polynomial fitting serves the purpose satisfactorily.

Purificator :

Since no process dynamics are considered for the purificator in this example, the production recipe for the purificator is given by Equation 2.38.

$$dur(2,2,n) = 2.0 \cdot vol(2,2,n) \tag{2.38}$$

Control Problem Formulation

The control problem is formulated using the standard production recipe, $i.e.$, Equations 2.36, 2.37 and 2.38, as per the continuous time formulation presented in section 2. However, within the control problem formulation Equations 2.36 and 2.37 have to be rewritten as Equations 2.39 and 2.40 respectively.

$$\begin{aligned} dur(1,1,n) = 1.743 \cdot te(1,n) + 1.172 \cdot vol(1,1,n) - 0.195 \cdot vol(1,1,n)^2 \\ +0.02518 \cdot vol(1,1,n)^3 \end{aligned} \tag{2.39}$$

$$Qr(1,1,n) = 0.1463 \cdot te(1,n) + 2.802 \cdot vol(1,1,n) - 0.05396 \cdot vol(1,1,n)^2 \tag{2.40}$$

The objective function for this example, which is maximization of overall profit for the plant, is expressed by Equation 2.41.

$$\begin{aligned} maximize \quad & \sum_n (180.0 \cdot d(3,n) - 60.0 \cdot vol(1,1,n) - 1.2 \cdot dur(1,1,n) \\ & -2.0 \cdot dur(2,2,n) - 4.0 \cdot Qr(1,1,n) - 75.0 \cdot vol(2,2,n)) \end{aligned} \tag{2.41}$$

Computational Result

A maximum profit of 30.8718 MU is achieved. A total amount of 2.637 m^3 of product is obtained by processing 2.93 m^3 of reactant and the corresponding production schedule is shown in Figure 2.4. The optimal solution converges for two event points and does not change with further increase in the number of event points. Throughout this work, the MINLP problems are solved using GAMS/SBB [2] solver on a Linux workstation with AMD Athlon(TM) XP 3200+ processor.

Control via the OOA

In the OOA, the process dynamics ($i.e.$, a set of Equations 2.30 - 2.34 for each task i in unit j at event point n) are directly included in the control model instead of the standard production recipe $i.e.$, Equations 2.36 - 2.38. The processing duration $dur(1, 1, n)$ and the energy resource requirement $Qr(1, 1, n)$ are obtained from the process dynamics included in the control problem.

Due to the direct consideration of the process dynamics, the control problem obtained in this case is a MIDO problem.

Computational Result

The MIDO problem is transformed into the MINLP problem by using standard trapezoidal rule with 100 equidistant time points. Two event points are needed for obtaining the optimal solution and the corresponding production schedule is shown in Figure 2.5. The optimal solution converges to a maximum profit value of 37.6109 MU and does not change with further increase in the number of event points. Figure 2.5 shows that this maximum profit is obtained by processing a total amount of 3.69 m^3 of the reactant, thereby producing 3.321 m^3 of the product.

Comparison of the Computational Results of the SRA and the OOA

Table 2.3 shows the model statistics and the solutions obtained via both the approaches. As expected, the size of the OOA control problem is very large (in terms of the number of variables and equations) in comparison to the SRA control problem and thus needs much

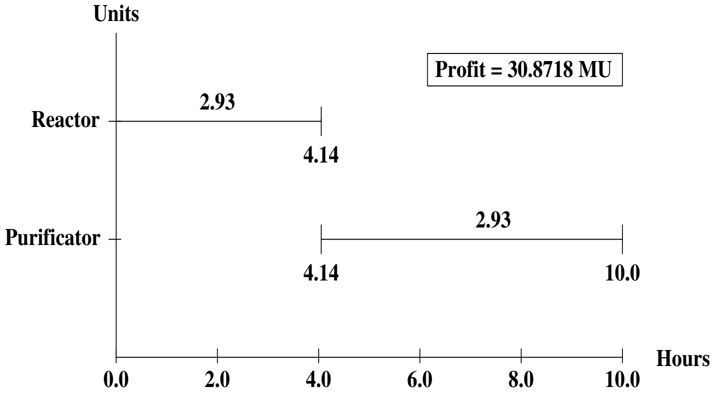

Figure 2.4: Optimal schedule obtained by the SRA for example 1.

more computational effort. However, the model statistics given for the SRA approach in Table 2.3 is only for the control problem. It should be noted that significant effort is involved in obtaining the standard recipe.

Table 2.3: Comparison of the SRA and the OOA results for example 1.

	SRA	OOA
Integer variables	2	2
Continuous variables	27	430
Equations	37	333
Solution (MU)	30.8718	37.6109

Nevertheless, in case of the OOA, the maximum profit increases by 21.83 %. Since the price of the product in this example is much higher than the other prices involved, the OOA control problem chooses to produce more product as quickly as possible while keeping all the other prices in check, which ultimately increases the overall profit for the plant significantly. The choice of this strategy by the OOA is possible only because of the additional degrees of freedom restored by the direct inclusion of the process dynamics in the control problem. To illustrate the influence of these additional degrees of freedom, let us consider the reaction task shown in Figure 2.5. The control profile followed by the OOA for this task is compared to that obtained by the SBO for the same batch size. These control profiles are shown in Figure 2.6 and the corresponding optimization results are shown in Table 2.4.

We see from Table 2.4 that for processing a volume of 3.69 m^3 the OOA takes 2.62 hours

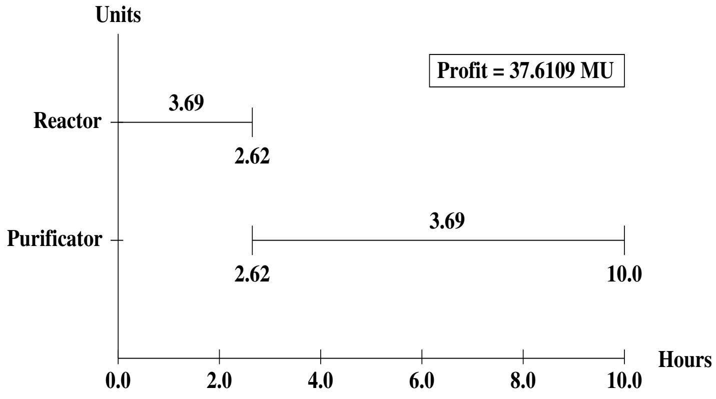

Figure 2.5: Optimal schedule obtained by the OOA for example 1.

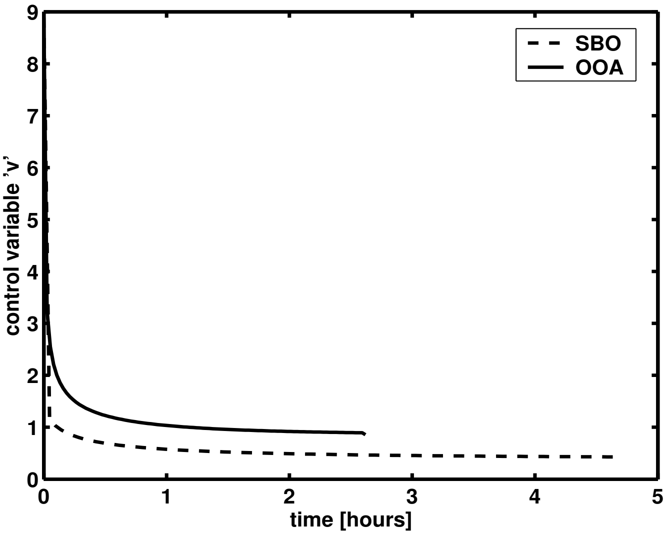

Figure 2.6: Control profiles for the reaction task (batch size 3.69 m^3) in example 1.

duration and 11.0366 units of energy resource, thereby corresponding to an operational cost of 47.2904 MU instead of the optimal 44.6453 MU obtained by the SBO. But this expensive mode of operation for the reaction task in the OOA allows more products to be produced during the entire process, thereby resulting in higher overall profit at the end of the time horizon. This clearly indicates that the OOA control problem is free to manipulate the control strategy so as to yield higher profit for the overall plant, rather than confining itself to the optimal control strategy obtained by the SBO.

Table 2.4: Optimization results for the reaction task (batch size 3.69 m^3) in example 1.

vol = 3.69 m^3		
	SBO	OOA
dur	4.6823	2.62
Qr	9.7566	11.0366
Cost (MU)	44.6453	47.2904

Influence of the SBO Objective Function

From the results obtained above, it seems that the results of the SRA can be easily improved by changing the objective for the SBO. Instead of minimizing the operation costs, we could minimize the operation costs per unit time or maximize the overall profit per unit time. This needs to be investigated and hence an alternate objective function is considered next for the SBO.

An Alternate Objective Function

Here, the objective function for the SBO is minimization of the operation cost for the reactor per unit time for a given batch size, as expressed by Equation 2.42.

$$minimize \quad \Big(\frac{operation\ cost\ for\ a\ given\ batch\ size\ (vol)}{duration\ of\ reaction\ (dur)}\Big) \tag{2.42}$$

subject to

$$Equations\ \text{2.30 - 2.34}$$

Where, the operation cost for a given batch size (vol) is given as follows :

$$Operation\ cost = 1.2 \cdot dur\ +\ 4.0 \cdot Qr \tag{2.43}$$

The SBO is performed for different batch sizes and the results are presented in Table 2.5. The SBO results presented in Table 2.5 show that the reaction duration dur and the specific heat requirement $Heat_f$ in this case are independent of the batch size. This is due to the particular objective function (Equation 2.42) chosen for the SBO. The common reaction recipe obtained for different batch sizes is shown in Figure 2.7.

Table 2.5: Results of the SBO for the alternate recipe.

vol(m^3)	$dur(hours)$	$Heat_f$	$Qr(m^3)$
2.0	2.3796	3.1492	6.2983
2.5	2.3796	3.1492	7.8729
3.0	2.3796	3.1492	9.4475
3.5	2.3796	3.1492	11.0221
4.0	2.3796	3.1492	12.5967
4.5	2.3796	3.1492	14.1713
5.0	2.3796	3.1492	15.7459

The standardized equations for the processing duration and energy requirement in terms of the control notation are given by Equations 2.44 & 2.45.

$$dur(1,1,n) = 2.3796 \cdot te(1,n), \quad \forall n\ \in\ N \tag{2.44}$$

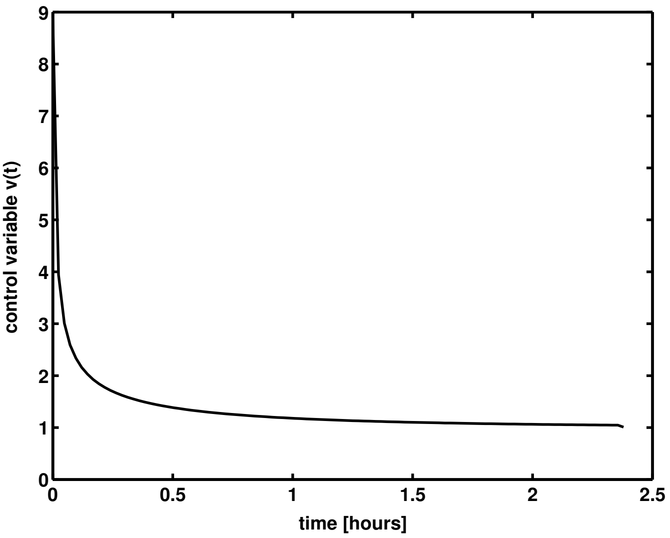

Figure 2.7: Optimal control profile for the reaction in alternative recipe case.

$$Qr(1,1,n) = 3.1492 \cdot vol(1,1,n), \quad \forall n \in N \tag{2.45}$$

Control via the SRA using the Alternate Recipe

The control problem presented in section 2.2.1 is solved again using the alternate recipe presented above. Since the duration of the reaction task is independent of the batch size, the control problem in this case is very trivial. The maximum profit for the plant in this case can be obtained simply by processing as much as possible within the given makespan. Hence, on a makespan of 10 hours a maximum of 3.8102 m^3 of reactant is processed in this example. Thus a maximum profit of 36.7862 MU is achieved with this

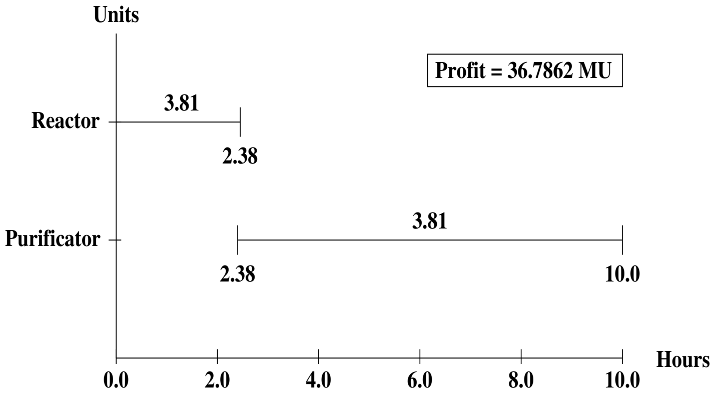

Figure 2.8: Optimal schedule obtained via the SRA using the alternate recipe.

alternate recipe and the corresponding production schedule is given in Figure 2.8.

On comparing Figure 2.8 with Figure 2.4, we see that with the alternate recipe the plant is able to produce more product within the given makespan, thereby yielding a higher profit. With this recipe the overall profit for the plant is very close to that obtained with the OOA. This gives the impression that this recipe is more appropriate for control via the SRA than the one used in section 2.2.1. However, this is not always the case, as illustrated next.

A fixed makespan of 25 hours is considered and the control problem is solved for this makespan. All the other information including the control objective and the recipes remain unchanged. The control problem is solved via the SRA (using both the recipes discussed above) as well as the OOA and the respective optimal production schedules are presented in Figures 2.9, 2.10 & 2.11.

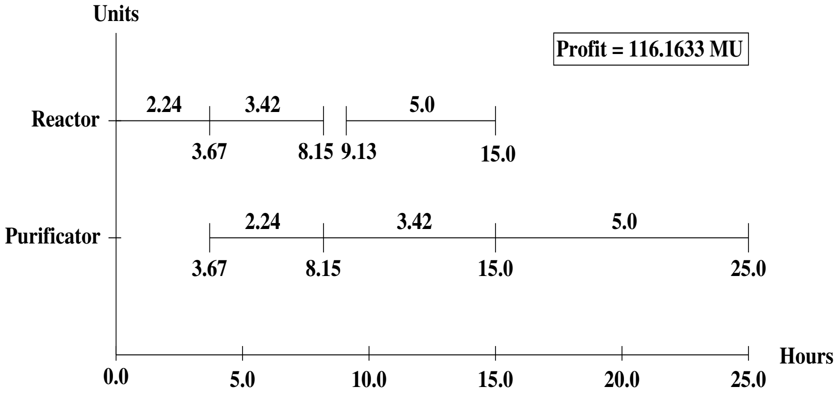

Figure 2.9: Optimal schedule obtained via the SRA using the first recipe (25 hours makespan).

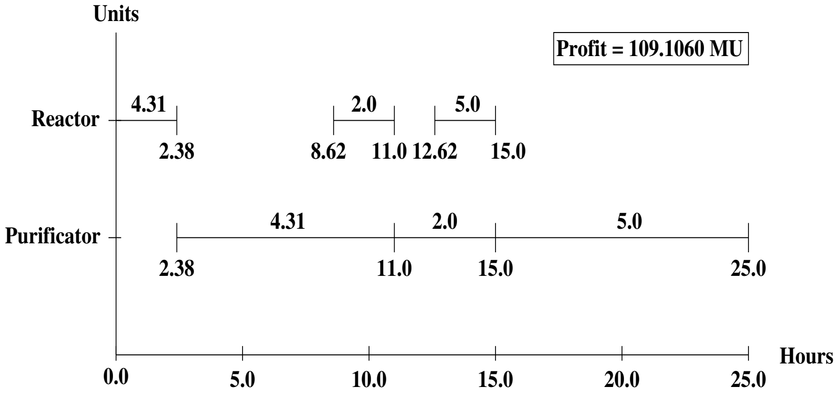

Figure 2.10: Optimal schedule obtained via the SRA using the alternate recipe (25 hours makespan).

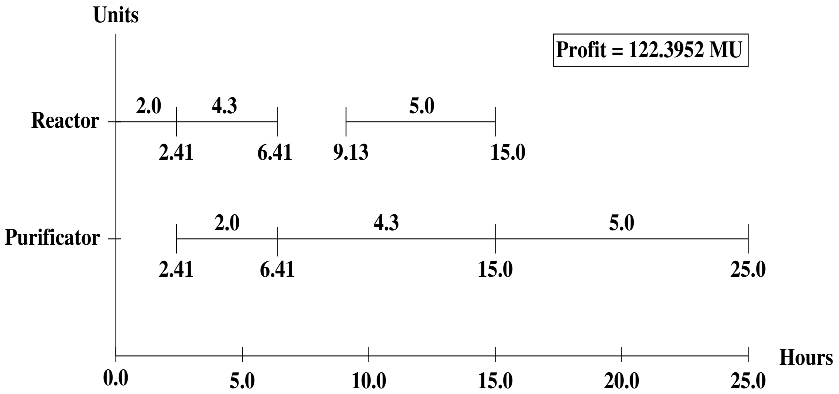

Figure 2.11: Optimal schedule obtained via the OOA (25 hours makespan).

Here, the overall profit obtained by using the alternate recipe is lower than that obtained by using the first recipe presented in section 2.2.1. Hence, in this case the alternate recipe which performed better than the first recipe on a makespan of 10 hours turns out to be a bad choice for the very same plant. However, this could not have been known in advance without executing the control problem with these recipes. As such, there are no standard rules available to obtain a recipe which would fetch the best overall optimal solution for a given plant and this is clearly a major drawback of the SRA. On the other hand, the overall profit obtained with the OOA is always better than that obtained with the SRA, as can be seen from Figures 2.5 & 2.11. The additional degrees of freedom due to the direct inclusion of the process dynamics in the control problem formulation indeed makes the OOA superior to the SRA. In principle, for any given plant, the OOA control problem is bound to be 'at least' as good as the SRA control problem in terms of the optimal solution obtained, provided it is computationally solvable.

Influence of the Process Cost Structure

The difference between the solutions obtained via the SRA and the OOA depends not only on the nature of the SBO objective function (e.g. minimization of operation costs or maximization of profit per unit time) but also on the values of the cost factors (i.e., parameters) in the SBO objective function, i.e., the cost *structure*. In practice, these depend on the process. For example, in pharmaceutical production, the materials are usually more expensive than the operating costs. This section illustrates the influence of different process cost structures on the difference in the control problem solutions obtained via both the approaches.

Let us consider different operation costs for the reactor while keeping all the other data unchanged. The SBO objective function chosen is the minimization of the operational costs, as presented in section 2.2.1. The control problem solutions obtained via both the approaches for these different cost structures on a makespan of 10 hours are presented in Table 2.6.

Table 2.6: Comparison of scheduling solutions for different reactor operation costs.

Reaction operation cost	SRA (MU)	OOA (MU)	improvement(%)
running cost = 1.2 $MU/hour$ energy resource cost = 4.0 MU/m^3	30.8718	37.6109	21.83
running cost = 2.6 $MU/hour$ energy resource cost = 2.6 MU/m^3	47.5210	50.2549	5.7530
running cost = 4.0 $MU/hour$ energy resource cost = 1.2 MU/m^3	63.3656	64.1516	1.24
running cost = 10.0 $MU/hour$ energy resource cost = 1.0 MU/m^3	52.7798	52.8733	0.1772

It is evident from the results presented in Table 2.6 that as the running cost of the reactor increases in comparison to the energy cost, the SRA control solution moves closer to the OOA control solution. This is due to the fact, that as the running cost of the reactor increases the SBO strategy tends to minimize processing time more than the energy requirement. This accordingly increases the amount of product being produced via the SRA control problem. Since the OOA control problem in this case also looks for producing as much as possible within the given time horizon, the difference in the SRA and the OOA control solutions decreases with the increasing running cost of the reactor in comparison to its energy cost.

However, the results presented in Table 2.6 are true only for the recipe chosen for the SRA and the given makespan of 10 hours. It may not hold true when different recipes are chosen and/or different makespan is considered, as discussed in section 2.2.1. Considering the fact that real chemical processes are characterized by much more complicated cost structures, it can be very challenging (or may be impossible) to choose an appropriate recipe for production control via the SRA. This problem can be eradicated with the

OOA, but the large size of the OOA control problems proves to be a major hindrance in its application to many real world problems.

2.2.2 Example 2

A multiple product plant consisting of two semi-batch reactors (R1 and R2) and three batch filters (F1, F2 and F3), as shown in Figure 1.1, is considered here. The plant is assumed to be operating under zero-wait policy. The processing stages involved are described in the following :

Reactors :

The reactors in the plant are dynamic semi-batch reactors with the following parallel reactions to be executed :

$$\begin{gathered} A_k \longrightarrow P_k \\ A_k \longrightarrow W_k \quad ; \qquad k = 1, 2, 3 \\ A_k = \text{reactant},\ P_k = \text{product},\ W_k = \text{waste} \end{gathered}$$

All the reactions are assumed to be carried out in the presence of a large amount of solvent. It is assumed that for every reaction the amount of solvent contributes 90 % of the given batch size. Before every reaction, the reactors are first filled with the required amount of solvent and then the reactants are dosed strategically.
The governing equations for the reactors are as follows :

$\forall k$

$$\frac{dX_{A_k}(t)}{dt} = F_{A_k}(t) \cdot C_{A_k} - (\alpha_k \cdot u_k(t)^{\beta_k} + u_k(t)) \cdot X_{A_k}(t) \; ; \quad X_{A_k}(t=0) \; = \; 0.0 \quad (2.46)$$

Where, C_{A_k} = 6.0 $kmoles/m^3$

$$\frac{dX_{P_k}(t)}{dt} = \alpha_k \cdot u_k(t)^{\beta_k} \cdot X_{A_k}(t) \; ; \quad X_{P_k}(t=0) \; = \; 0.0 \quad (2.47)$$

$$\frac{dX_{W_k}(t)}{dt} = u_k(t) \cdot X_{A_k}(t) \; ; \quad X_{W_k}(t=0) \; = \; 0.0 \quad (2.48)$$

$$\frac{dV_k(t)}{dt} = F_{A_k}(t) \; ; \quad V_k(t=0) \; = \; 0.9 \cdot vol_k \; ; \; V_k(t=dur_k) \; = \; vol_k \quad (2.49)$$

$$Qr_k = \int_0^{dur_k} u_k(t) \cdot dt \tag{2.50}$$

$$X_{A_k}(t) \;\leq\; 2.0\, kmoles \tag{2.51}$$

$$0.01\, hour^{-1} \;\leq\; u_k(t) \;\leq\; 4.0\, hour^{-1} \tag{2.52}$$

$$F_{A_k}(t) \;\leq\; 0.5\, m^3/hour \tag{2.53}$$

$$X_{P_k}(t = dur_k) = 0.9 \cdot (0.1 \cdot vol_k \cdot C_{A_k}) \tag{2.54}$$

Where, $X_{A_k}(t)$, $X_{P_k}(t)$ and $X_{W_k}(t)$ represent the moles of reactant A_k, product P_k and waste W_k respectively at any instant of time t ($t \in [0,\ dur_k]$), while their respective rate equations are given by Equations 2.46, 2.47 and 2.48. α_k and β_k are kinetic parameters for the reactions and are given in Table 2.7. $u_k(t)$ is a rate constant, which is assumed to be a control variable. $F_{A_k}(t)$ is also a control variable, which represents the feed flow rate of reactant A_k at any instant of time t. C_{A_k} represents the concentration of reactant A_k in the feed. vol_k is the batch size for the given reaction in m^3. The minimum batch size required for a reactor to operate is assumed to be 20 % of the maximum capacity of that reactor. $V_k(t)$ represents the volume of the reacting mixture at any instant of time t and its rate of change due to the addition of reactant A_k is given by Equation 2.49. The initial condition for Equation 2.49 corresponds to the fact that before every reaction the reactors are filled with the required amount of solvent, $i.e.$, 90 % of the given batch size. Qr_k represents the energy resource requirement for the reaction, which is given by the integral over $u_k(t)$ as per Equation 2.50. Equations 2.51, 2.52 and 2.53 represent path constraints, mainly for safe operation of the reactors. Equation 2.54 represents an end constraint, which expresses that the operational yield of the product at the end of the reaction should be 90 %.

Table 2.7: Kinetic parameters for the reactions in example 2.

k	1	2	3
$\alpha_k(hour^{\beta_k - 1})$	2	2	3
β_k	0.5	0.4	0.5

Filters :

The filters in the plant are assumed to be batch filters. The intermediates from the reactors are sent to the filters, where the solvent is totally recovered and the rest is sent out as products. The following assumptions are made for the operation of the filters :

1. The time needed for filtration is given by the following :
   filtration duration ($hours$) = 1.2 $\cdot$ (volume of intermediate being purified (m^3))
2. The intermediate is split volumetrically into the solvent (90 %) and the final product (10 %). Note that the final product in this case is a mixture of the product P_k, the waste W_k and the unreacted reactant A_k.

The STN representation of the process is shown in Figure 1.2, while the basic data for the units and the states is presented in Table 2.8. The running cost of the reactors and the filters as well as the energy resource cost for the reactors remain exactly the same as in Example 1. Whereas, the cost of resources needed for every filtration is assumed to be 20.0 MU per m^3 of the intermediate being processed.

Table 2.8: Data for example 2.

Unit(j)	Capacity(m^3)	Suitability(task i)
Reactor R1(j=1)	2.0	Reactions 1(i=1), 2(i=3) & 3(i=5)
Reactor R2(j=2)	1.0	Reactions 1(i=2), 2(i=4) & 3(i=6)
Filter F1(j=3)	1.0	Filtrations 1(i=7), 2(i=10) & 3(i=13)
Filter F2(j=4)	1.0	Filtrations 1(i=8), 2(i=11) & 3(i=14)
Filter F3(j=5)	1.0	Filtrations 1(i=9), 2(i=12) & 3(i=15)
State(s)	**initial amount(m^3)**	**price(MU per m^3)**
Reactant A_1(s=1)	20.0	40.0
Reactant A_2(s=2)	20.0	35.0
Reactant A_3(s=3)	20.0	25.0
Intermediate 1(s=4)	0.0	0.0
Intermediate 2(s=5)	0.0	0.0
Intermediate 3(s=6)	0.0	0.0
Product 1(s=7)	0.0	430.0
Product 2(s=8)	0.0	410.0
Product 3(s=9)	0.0	385.0
Solvent(s=10)	40.0	2000.0

The objective for this example is maximization of overall profit for the plant over a fixed makespan of 7 hours, where the overall profit for the plant is defined as follows :

$$\begin{aligned} Profit &= (price\ of\ products) - (price\ of\ reactants) \\ &- (cost\ of\ resources\ needed\ for\ filtration) \\ &- (energy\ resource\ cost\ of\ the\ reactors) \\ &- (running\ cost\ of\ the\ reactors) \\ &- (running\ cost\ of\ the\ filters) \end{aligned}$$

The minimum production requirement for each product in order to satisfy the market demand is assumed to be 0.06 m^3. Also it is assumed that without cleaning requirements the filters can only be used for filtering in the sequence Intermediate 1, 2 and 3. If this sequence cannot be followed on a particular filter then a cleaning time of one hour is needed for that filter before filtering the following intermediate. However, apart from the cleaning time no other cost is assumed for cleaning the filters.

Control via the SRA

Determination of Standard Production Recipe

Reactors :
The standard production recipe for the reactors (for producing each product) in this example involves determination of the optimal heating and dosing policy, which is done via single batch optimization (SBO) for the respective reaction. Since for a given batch size with fixed operational yield maximum profit can be achieved by minimization of the operational cost of the reactors, it is chosen as the SBO objective. The SBO problem can be written as follows :

$$minimize \quad (1.2 \cdot dur_k + 4.0 \cdot Qr_k) \tag{2.55}$$

subject to

$$Equations \quad \text{2.46 - 2.54}$$

The SBO for each reaction is carried out for different batch sizes using 100 equidistant time points and the corresponding results are presented in Tables 2.9, 2.10 and 2.11. The standardized equations for processing duration and energy resource requirement for each reaction in terms of the control notation, as given by Equation 2.56, are obtained

Table 2.9: SBO results for reaction 1 in example 2.

$vol_1(m^3)$	Qr_1	$dur_1(hours)$
0.2	0.4493	4.5560
0.4	0.4493	4.5770
0.6	0.4509	4.6346
0.8	0.4675	4.8830
1.0	0.4967	5.2279
1.2	0.5304	5.6316
1.4	0.5689	6.0612
1.6	0.6107	6.5073
1.8	0.6551	6.9635
2.0	0.7018	7.4260

by suitably fitting the data shown in Tables 2.9, 2.10 and 2.11 with polynomials of appropriate order.

$$\begin{aligned} dur(1,1,n) = 4.75 \cdot te(1,n) - 1.35 \cdot vol(1,1,n) + 2.3 \cdot vol(1,1,n)^2 \\ -0.48 \cdot vol(1,1,n)^3 \end{aligned}$$

Table 2.10: SBO results for reaction 2 in example 2.

$vol_2(m^3)$	Qr_2	$dur_2(hours)$
0.2	0.2869	3.2896
0.4	0.2874	3.3089
0.6	0.2888	3.3508
0.8	0.3033	3.5187
1.0	0.3247	3.7685
1.2	0.3521	4.0558
1.4	0.3836	4.3644
1.6	0.4179	4.6877
1.8	0.4555	5.0159
2.0	0.4969	5.3465

Table 2.11: SBO results for reaction 3 in example 2.

$vol_3(m^3)$	Qr_3	$dur_3(hours)$
0.2	0.3200	2.3259
0.4	0.3198	2.3486
0.6	0.3220	2.3815
0.8	0.3362	2.4991
1.0	0.3610	2.6601
1.2	0.3899	2.8515
1.4	0.4227	3.0565
1.6	0.4588	3.2681
1.8	0.5000	3.4756
2.0	0.5402	3.6986

$$dur(2,2,n) = 4.75 \cdot te(2,n) - 1.35 \cdot vol(2,2,n) + 2.3 \cdot vol(2,2,n)^2 \\ -0.48 \cdot vol(2,2,n)^3$$

$$Qr(1,1,n) = 0.47 \cdot te(1,n) - 0.132 \cdot vol(1,1,n) + 0.193 \cdot vol(1,1,n)^2 \\ -0.0344 \cdot vol(1,1,n)^3$$

$$Qr(2,2,n) = 0.47 \cdot te(2,n) - 0.132 \cdot vol(2,2,n) + 0.193 \cdot vol(2,2,n)^2 \\ -0.0344 \cdot vol(2,2,n)^3$$

$$dur(3,1,n) = 3.43 \cdot te(3,n) - 0.963 \cdot vol(3,1,n) + 1.64 \cdot vol(3,1,n)^2 \\ -0.339 \cdot vol(3,1,n)^3$$

$$dur(4,2,n) = 3.43 \cdot te(4,n) - 0.963 \cdot vol(4,2,n) + 1.64 \cdot vol(4,2,n)^2 \\ -0.339 \cdot vol(4,2,n)^3$$

$$Qr(3,1,n) = 0.301 \cdot te(3,n) - 0.0924 \cdot vol(3,1,n) + 0.137 \cdot vol(3,1,n)^2 \\ -0.0211 \cdot vol(3,1,n)^3$$

$$Qr(4,2,n) = 0.301 \cdot te(4,n) - 0.0924 \cdot vol(4,2,n) + 0.137 \cdot vol(4,2,n)^2 \\ -0.0211 \cdot vol(4,2,n)^3$$

$$\begin{aligned} dur(5,1,n) &= 2.4 \cdot te(5,n) - 0.556 \cdot vol(5,1,n) + 1.02 \cdot vol(5,1,n)^2 \\ &\quad -0.212 \cdot vol(5,1,n)^3 \\ dur(6,2,n) &= 2.4 \cdot te(6,n) - 0.556 \cdot vol(6,2,n) + 1.02 \cdot vol(6,2,n)^2 \\ &\quad -0.212 \cdot vol(6,2,n)^3 \\ Qr(5,1,n) &= 0.336 \cdot te(5,n) - 0.107 \cdot vol(5,1,n) + 0.157 \cdot vol(5,1,n)^2 \\ &\quad -0.0265 \cdot vol(5,1,n)^3 \\ Qr(6,2,n) &= 0.336 \cdot te(6,n) - 0.107 \cdot vol(6,2,n) + 0.157 \cdot vol(6,2,n)^2 \\ &\quad -0.0265 \cdot vol(6,2,n)^3 \end{aligned} \tag{2.56}$$

Purificators :
Once again no process dynamics are considered for the tasks of purification and hence the production recipe for the purificators is given by the Equations 2.57 - 2.59.

$$dur(i,3,n) = 1.2 \cdot vol(i,3,n), \quad \forall i \in \{7,10,13\} \tag{2.57}$$

$$dur(i,4,n) = 1.2 \cdot vol(i,4,n), \quad \forall i \in \{8,11,14\} \tag{2.58}$$

$$dur(i,5,n) = 1.2 \cdot vol(i,5,n), \quad \forall i \in \{9,12,15\} \tag{2.59}$$

Control Problem Formulation
The control problem is formulated using the standard production recipe, $i.e.$, Equations 2.56 - 2.59. The objective function, which is maximization of overall profit for the plant, is expressed by Equation 2.60.

$$
\begin{aligned}
maximize \qquad & \sum_n (430.0 \cdot d(7,n) + 410.0 \cdot d(8,n) \\
& +385.0 \cdot d(9,n) - 40.0 \cdot (0.1 \cdot (vol(1,1,n) + vol(2,2,n))) \\
& -35.0 \cdot (0.1 \cdot (vol(3,1,n) + vol(4,2,n))) - 25.0 \cdot (0.1 \cdot (vol(5,1,n) \\
& +vol(6,2,n))) - 1.2 \cdot (dur(1,1,n) + dur(2,2,n) \\
& +dur(3,1,n) + dur(4,2,n) + dur(5,1,n) + dur(6,2,n)) \\
& -2.0 \cdot (dur(7,3,n) + dur(8,4,n) + dur(9,5,n) + dur(10,3,n) \\
& +dur(11,4,n) + dur(12,5,n) + dur(13,3,n) + dur(14,4,n) \\
& +dur(15,5,n)) - 4.0 \cdot (Qr(1,1,n) + Qr(2,2,n) + Qr(3,1,n) \\
& +Qr(4,2,n) + Qr(5,1,n) + Qr(6,2,n)) - 20.0 \cdot (vol(7,3,n) \\
& +vol(8,4,n) + vol(9,5,n) + vol(10,3,n) + vol(11,4,n) \\
& +vol(12,5,n) + vol(13,3,n) + vol(14,4,n) + vol(15,5,n))) \qquad (2.60)
\end{aligned}
$$

Computational Result
A maximum profit of 31.9093 MU is achieved and the corresponding production schedule is shown is Figure 2.12. The optimal solution converges for five event points and does not change with further increase in the number of event points.

Control via the OOA

The OOA control problem directly involves the process dynamics given by Equations 2.46 - 2.54 instead of the standard production recipe for the products.

Computational Result
Once again 100 equidistant time points were used to transform the underlying MIDO problem into a MINLP problem. A profit of 36.5287 MU is obtained by using four event points and the corresponding production schedule is shown in Figure 2.13. It could not be checked whether the profit increases further with increase in the number of event points, as a further increase in the number of event points renders the control problem insolvable in acceptable computation time.

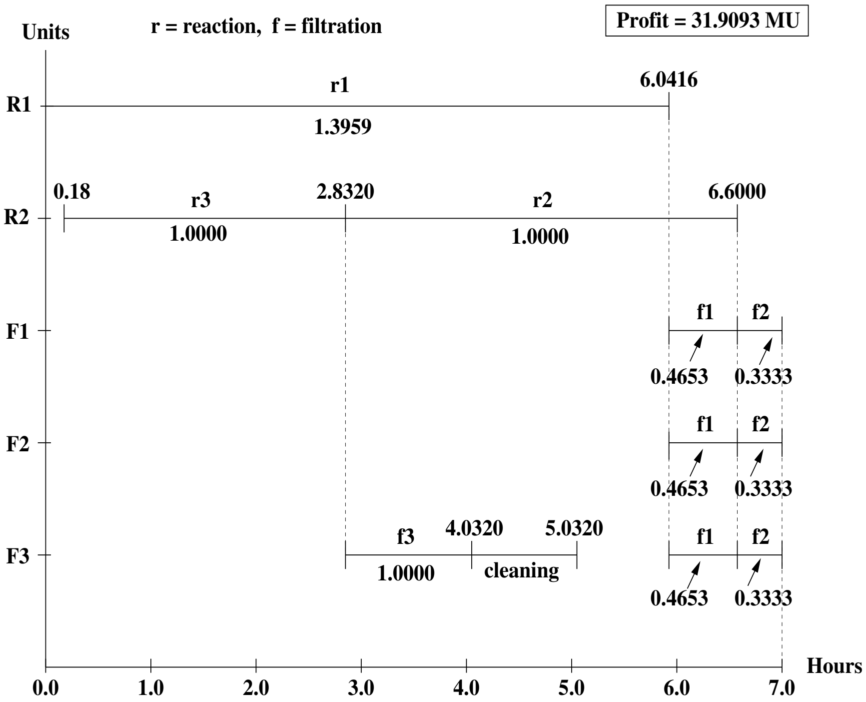

Figure 2.12: Optimal schedule obtained by the SRA for example 2.

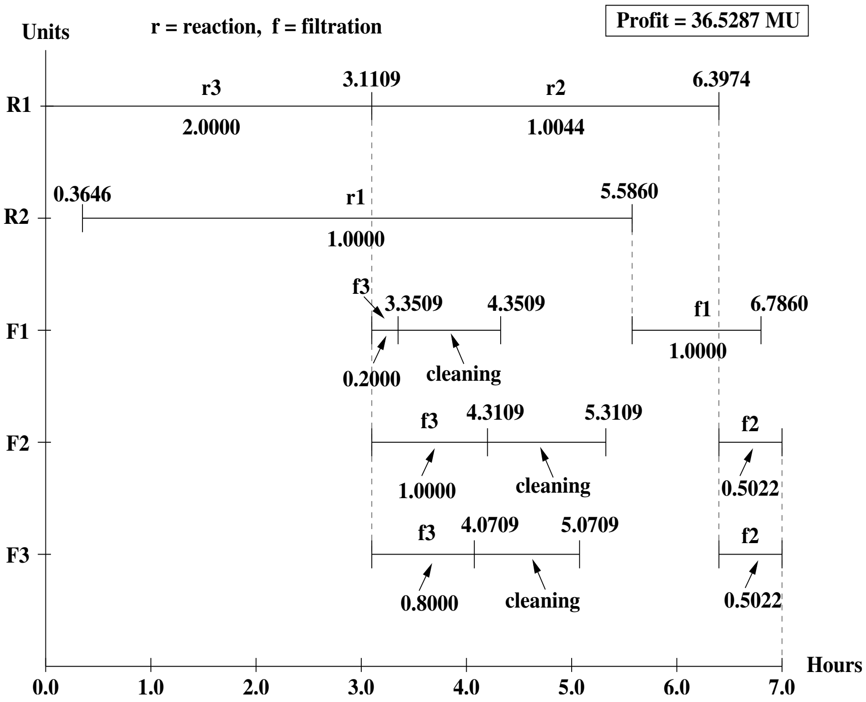

Figure 2.13: Optimal schedule obtained by the OOA for example 2.

Comparison of the Computational Results of the SRA and the OOA

The model statistics and the solutions obtained via both the approaches for this example are presented in Table 2.12. It is observed that the overall profit for the plant obtained via the OOA is 14.48 % higher than that obtained with the SRA. Once again, this can be attributed to the ability of the OOA control problem to manipulate the control policy instead of adhering to the control strategy obtained by the SBO, as shown in Table 2.13. The results presented in Table 2.13 show that the OOA control problem chooses an expensive mode of operation for the reactors instead of the more economical mode of operation obtained by the SBO. However, like in example 1, this expensive mode of operation reduces processing time on the reactors, which finally allows more production over the entire makespan thereby increasing the overall profit for the plant. It should be noted that the SRA solution presented in Table 2.12 is subject to the SBO objective function chosen, as discussed in section 2.2.1.

The model statistics presented in Table 2.12 clearly show that the size of the OOA control problem in this case is much larger than its SRA counterpart, thereby making it computationally very expensive. The computation time needed for the OOA control problem in this case is roughly 29 times higher than that needed for the corresponding SRA control problem. Moreover, the OOA model statistics and solution presented in Table 2.12 correspond only to four event points. A further increase in the number of event points makes the OOA control problem too difficult to be solved in acceptable computation time, as presented in Table 2.14. This clearly indicates the inapplicability of the OOA to larger chemical plants, thereby advocating the need for novel solution techniques for such problems.

Table 2.12: Comparison of the SRA and the OOA results for example 2.

	SRA	OOA
Integer variables	75	60
Continuous variables	441	12969
Equations	1143	9864
Solution (MU)	31.9093	36.5287
CPU time(s)	99.53	2885.85

Table 2.13: Comparison of the reactor operation cost followed by the OOA scheduling model and that obtained via SBO for example 2.

Reaction	batch size (m^3)	OOA	SBO
r1	1.0000	dur_1 = 5.2214 (hours) Qr_1 = 0.4990 operation cost = 8.2617 (MU)	dur_1 = 5.2279 (hours) Qr_1 = 0.4967 operation cost = 8.2604 (MU)
r2	1.0044	dur_2 = 3.2865 (hours) Qr_2 = 0.6761 operation cost = 6.6482 (MU)	dur_2 = 3.7746 (hours) Qr_2 = 0.3253 operation cost = 5.8307 (MU)
r3	2.0000	dur_3 = 3.1109 (hours) Qr_3 = 0.9484 operation cost = 7.5267 (MU)	dur_3 = 3.6986 (hours) Qr_3 = 0.5402 operation cost = 6.5990 (MU)

Table 2.14: OOA scheduling model statistics for example 2 with 5 event points.

Integer variables	75
Continuous variables	17258
Equations	13100
Solution (MU)	terminated before completion
CPU time(s)	$>$ 184125

2.3 Summary

In this chapter, two major approaches, $i.e.$, the SRA and the OOA, are applied to a control problem of chemical processes and their performance is compared. It is shown that the results obtained with the SRA can be suboptimal due to standardization of the production recipes, which remove degrees of freedom from the system. Moreover, this approach is clouded by ambiguities concerning the determination of the standard production recipes, as discussed in section 2.2.1. On the other hand, the OOA does not need standard recipes at all for production control and hence it is free from all the problems associated with the standard recipe determination. Moreover, due to relatively more degrees of freedom this approach results in solutions which are at least as good as that obtained with the SRA.

In terms of the solutions obtained, the OOA is definitely superior to the SRA. But there are some severe drawbacks which make this approach unfavorable for many real world problems. The major drawback comes from the fact that the MINLP problems obtained via discretization of the underlying MIDO problem are usually very large in size and hence computationally very difficult or even impossible for problems involving large chemical plants, as seen in section 2.2.2. This problem is further aggravated if the unit operations in the plant involve discrete/hybrid process dynamics, because for such plants the number of integer variables in the OOA control problem can be very high.

Nevertheless, considering the potential for significantly better solutions, the OOA approach needs to be focused upon. Novel solution techniques need to be developed to tackle the major challenges (particularly the size and the non-convexity of the control problems) posed by this approach, especially for plants involving discrete/hybrid unit operations. A natural line for future research is therefore to establish "smart" decomposition techniques which, by imposing suitable solution structure, reduce degrees of freedom while only minimally affecting achievable performance. In this way, one may hope to recover the solution theoretically obtainable by the OOA more closely than by the SRA while keeping a lid on complexity. This forms the basis of the next chapter.

Chapter 3

An Improved Approach for the Control of Multiproduct Batch Plants

The comparative study presented in chapter 2 clearly indicates that the SRA results in solutions that are usually far from the optimal. However, the control problems obtained with this approach can be solved conveniently with the conventional solvers readily available in the market. The OOA, on the other hand, results in solutions that are usually far better than that obtained with the SRA. But, the control problems obtained with this approach are computationally very difficult, which renders this approach inapplicable to the problems of practical size. This advocates the need for a better approach, which has computational features like the control problems obtained via the SRA and degrees of freedom like the control problems obtained via the OOA, as depicted in Figure 3.1.

Figure 3.1: An improved approach for the control of MBPs.

In the SRA, the control problem is parameterized by a recipe with only one free parameter, that is, the batch size $vol(i, j, n)$. A straightforward extension to this approach is to use more than one free parameter for the parameterization of the control problem. This will add further degrees of freedom to the control problem without requiring the direct inclusion of the process dynamics, as in the OOA. This brings us to the improved approach that is proposed next.

Kindly note that in this work we restrict to introducing just two free parameters for the parameterization of the control problem, as it is enough for the examples considered here. Besides, introduction of more than two free parameters would not only make the recipes quite cumbersome to obtain but also very difficult to visualize.

3.1 Control of MBPs via the Improved Approach

The IA for the control of MBPs involves determination of suitable recipe functions followed by the control problem formulation on the basis of these functions.

3.1.1 Determination of suitable recipe functions

The suitable recipe functions are determined via single batch optimization (SBO). However, unlike the SRA, the following two different types of SBO problems are solved in this case for different batch sizes and for every task on a given unit.

SBO problem 1 :

This SBO problem involves determination of the minimum processing durations dur_0 for different batch sizes and for all tasks on all units.

$$minimize \qquad dur_0, \quad \forall i \in I, \; j \in J_i, \; n \in N \tag{3.1}$$

subject to

$$Equations \quad \text{2.21 - 2.27}$$

where, $t \in [0, dur_0]$ and $t_{ep} \in \{0, dur_0\}$

This problem is solved for different batch sizes and all tasks on all units and the corresponding dur_0 are obtained as in Table 3.1. The dependence of the minimum processing duration $dur_0(i, j, n)$ on the batch size $vol(i, j, n)$ for every task i in unit j at event point n, as given by Equation 3.2, is then obtained via suitable polynomial fitting of the data in Table 3.1.

$$dur_0(i,j,n) = \begin{cases} 0, & vol(i,j,n) = 0 \\ \pi_1(vol(i,j,n)), & vol(i,j,n) > 0 \end{cases} \tag{3.2}$$

Table 3.1: Minimum processing durations for different batch sizes for a given task in a given unit.

vol	$dur_0\ (for\ vol)$
vol_1	$dur_0\ (for\ vol_1)$
vol_2	$dur_0\ (for\ vol_2)$
$\vdots$	$\vdots$
vol_{last}	$dur_0\ (for\ vol_{last})$

SBO problem 2 :

This SBO problem involves determination of the minimum resources Qr required over different processing durations for a given batch size and for all tasks on all units.

$$minimize \qquad Qr, \quad \forall i \in I,\ j \in J_i,\ n \in N \tag{3.3}$$

subject to

$$Equations \quad \text{2.21 - 2.27}$$

where, $t \in [0, dur]$, $t_{ep} \in \{0, dur\}$ and $dur > dur_0$

This problem is solved and for different batch sizes and every task on a given unit, a family of optimal control profiles is obtained over the time domain of interest, as illustrated in Table 3.2.

Table 3.2: Data corresponding to optimal control profiles for different batch sizes and a given task on a given unit.

vol_1		vol_2		$\dots$	vol_{last}	
dur	Qr	dur	Qr	$\dots$	dur	Qr
dur_0	Qr_0	dur_0	Qr_0	$\dots$	dur_0	Qr_0
dur_1	Qr_1	dur_1	Qr_1	$\dots$	dur_1	Qr_1
dur_2	Qr_2	dur_2	Qr_2	$\dots$	dur_2	Qr_2
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\dots$	$\vdots$	$\vdots$
dur_{last}	Qr_{last}	dur_{last}	Qr_{last}	$\dots$	dur_{last}	Qr_{last}

The data in Table 3.2 is then used to determine the remaining suitable recipe functions, that are given by Equation 3.2 and Equations 3.4 - 3.6.
$\forall i \in I,\ j \in J_i,\ n \in N$

$$Qr(i,j,n) = \begin{cases} 0, & vol(i,j,n) = 0 \\ \pi_2(vol(i,j,n), dur(i,j,n)), & vol(i,j,n) > 0 \end{cases} \tag{3.4}$$

$$dur(i,j,n) = 0, \quad \forall\, vol(i,j,n) = 0 \tag{3.5}$$

$$dur(i,j,n) \geq dur_0(i,j,n) \ + \ \delta(i,j,n), \quad \forall\, vol(i,j,n) > 0 \tag{3.6}$$

Equation 3.4 is obtained via suitable polynomial regression of the data given in table 3.2. Equations 3.5 and 3.6 ensure that whenever a task is being executed, the processing duration for that should not be less than the minimum processing duration dur_0 required for that task for the given batch size. The $\delta(i,j,n)$ in Equation 3.6 is a correction factor, which is obtained from Figure 3.2 as follows:

$\delta(i,j,n)$ = the absolute minimum of all "residuals" that are less than zero.
where, residual = fitted $dur_0(i,j,n)$ - true $dur_0(i,j,n)$

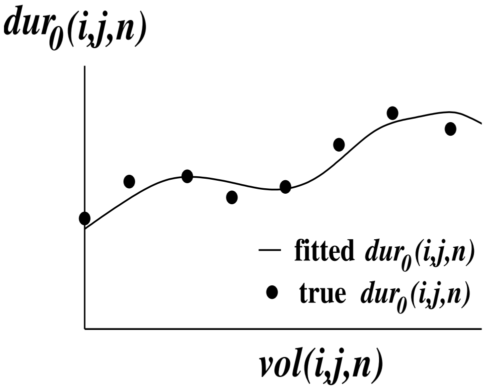

Figure 3.2: An illustration of the polynomial fitting used for obtaining Equation 3.2.

$\delta(i,j,n)$ allows Equation 3.6 to ensure that the processing duration obtained with it is never less than the minimum processing duration that is physically possible for the given task on a given unit.

It needs to be mentioned that the orders of polynomial fittings used for obtaining Equations 3.2 and 3.4 have to be chosen very carefully, as the data used for obtaining these equations can be highly nonlinear or non-smooth. Besides, they should be such that no further computational difficulties are introduced, while at the same time keeping a check on the residuals.

3.1.2 Control problem formulation

The control problem is then formulated using Equations 3.2 - 3.6 instead of the process dynamics. The resulting control problem in this case is either a MILP or a MINLP problem depending on whether Equations 3.2, 3.4 and the objective function are linear or nonlinear respectively.

3.2 Illustrative examples

In this section, the illustrative examples considered in chapter 2 are reconsidered. The IA is applied to these examples and the results obtained thereby are compared with the results obtained via the SRA and the OOA for these examples.

3.2.1 Example 1

The single product plant presented in section 2.2.1 is reconsidered here. The process flowsheet, the corresponding STN, the governing equations for the units and all the other data remain exactly the same as in 2.2.1. The objective of the control problem is maximization of the overall profit for the plant over a makespan of 25 hours. The control problem, as discussed in the previous section, involves determination of suitable recipe functions followed by the control problem formulation on the basis of these functions.

Determination of suitable recipe functions

Reactor :
The suitable recipe functions for the reactor are determined via solution of the following two SBO problems.

SBO problem 1
This step involves determination of the minimum processing durations for different

batch-sizes by solving the following SBO problem:

$$minimize \quad dur_0 \tag{3.7}$$

subject to

$$Equations \ \ 2.30 \text{ - } 2.34$$

The SBO is carried out using the standard trapezoidal rule with 100 equidistant time points. The corresponding results are furnished in Table 3.3 and the corresponding control profile is shown in Figure 3.3.

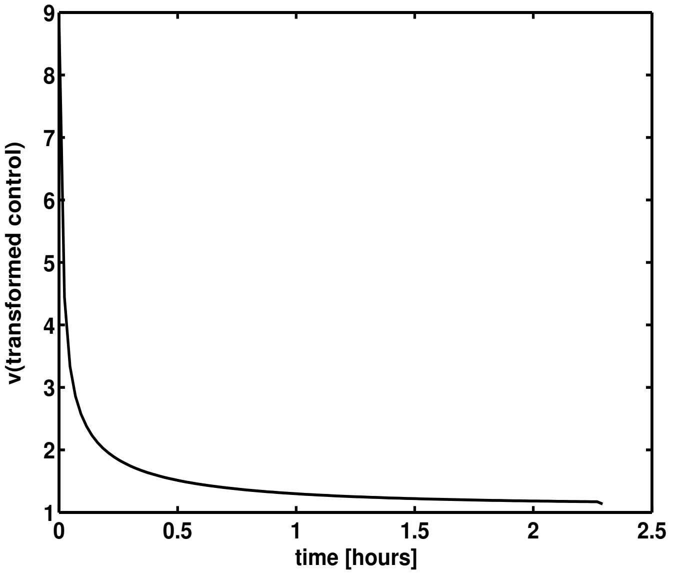

Figure 3.3: Optimal control profile corresponding to the minimum processing time for the reaction in example 1.

From the results presented in Table 3.3, we see that, for this example, the minimum processing duration remains the same for all the batch sizes. This is due to the simple governing equations chosen for this example.

The dependence of the minimum processing duration on the batch size is very straightforward in this case and is expressed by Equation 3.8.

$$dur_0(1,1,n) = \begin{cases} 0, & vol(1,1,n) = 0 \\ 2.2921, & vol(1,1,n) > 0 \end{cases} \tag{3.8}$$

Table 3.3: Minimum processing durations for different batch sizes for the reaction in example 1.

$vol\ (m^3)$	$dur_0\ (hours)\ (for\ vol)$
2.0	2.2921
2.5	2.2921
3.0	2.2921
$\vdots$	$\vdots$
5.0	2.2921

SBO problem 2

The minimum energy resource Qr required over different processing durations for different batch-sizes on the reactor is determined in this step via the following SBO problem. The results obtained thereby are presented in Table 3.4.

$$minimize \quad Qr \tag{3.9}$$

subject to

$$Equations \ \ 2.30 \text{ - } 2.34$$

Table 3.4: Data corresponding to optimal control profiles for different batch sizes and for the reaction in example 1.

2.0 m^3		2.5 m^3		…	5.0 m^3	
dur $(hours)$	Qr (m^3)	dur $(hours)$	Qr (m^3)	…	dur $(hours)$	Qr (m^3)
2.2921	6.7256	2.2921	8.4070	…	2.2921	16.8140
2.75	5.8752	2.75	7.3440	…	2.75	14.6880
3.25	5.6244	3.25	7.0305	…	3.25	14.0610
$\vdots$	$\vdots$	$\vdots$	$\vdots$	…	$\vdots$	$\vdots$
17.25	3.4254	17.25	4.2818	…	17.25	8.5635

Figure 3.4 presents the optimal control profiles corresponding to minimum Qr required for processing a batch-size of 2.5 m^3 over different time durations. For the sake of brevity, the optimal control profiles for the other batch-sizes are not presented here.

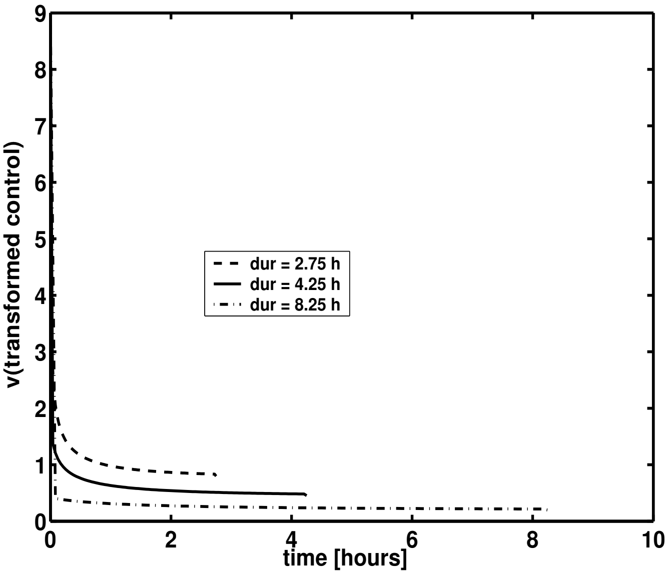

Figure 3.4: Optimal control profiles (u) corresponding to different processing durations for a batch-size of 2.5 m^3 in example 1.

The remaining recipe functions, as given by Equations 3.10 - 3.12, are then determined by using the data presented in Table 3.4.

$$Qr(1,1,n) = \begin{cases} 0, & vol(1,1,n) = 0 \\ (1.9674 + 3.4719 \cdot vol(1,1,n) & \\ -0.8633 \cdot dur(1,1,n) + 0.0633 \cdot vol(1,1,n)^2 & \\ -0.2050 \cdot vol(1,1,n) \cdot dur(1,1,n) & \\ +0.1162 \cdot dur(1,1,n)^2 - 0.0043 \cdot vol(1,1,n)^3 & \\ +0.0016 \cdot vol(1,1,n)^2 \cdot dur(1,1,n) & \\ +0.0046 \cdot vol(1,1,n) \cdot dur(1,1,n)^2 & \\ -0.0041 \cdot dur(1,1,n)^3), & vol(1,1,n) > 0 \end{cases} \tag{3.10}$$

$$dur(1,1,n) = 0, \quad \forall\, vol(1,1,n) = 0 \tag{3.11}$$

$$dur(1,1,n) \geq dur_0(1,1,n) \; + \; \delta(1,1,n), \quad \forall\, vol(1,1,n) > 0 \tag{3.12}$$

where, $\delta(1,1,n)$ = 0.0

Equation 3.10 is obtained via third order polynomial regression of the data presented in Table 3.4. Figure 3.5, shows the plot of the polynomial obtained in Equation 3.10. It is clear from Figure 3.5 that the obtained polynomial is very smooth and not liable to introduce any further computational difficulty in the control problem. Equations 3.11 and

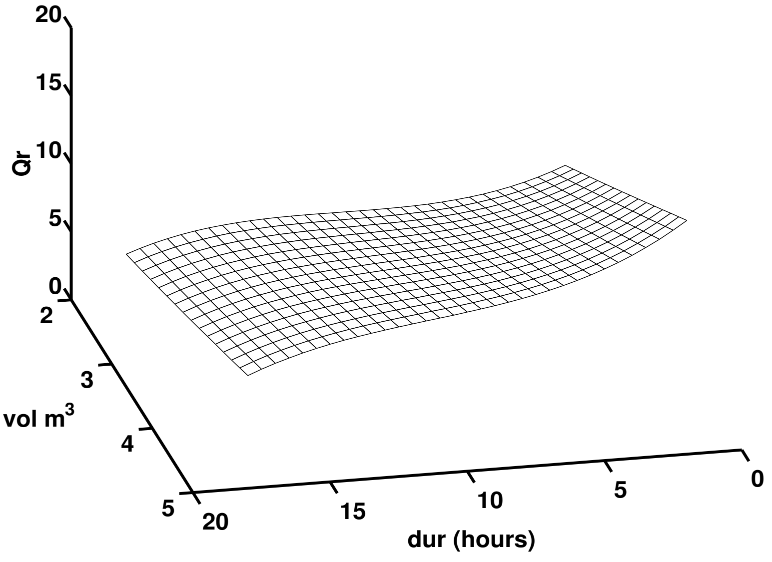

Figure 3.5: Plot of the third order polynomial given in Equation 3.10.

3.12 ensure that whenever a reaction is taking place on the reactor, the processing duration needed for it should not be less than the minimum duration required for processing the given batch size. Note that the correction factor δ in this case is zero, as Equation 3.8 involves just a single value and therefore, has no residuals associated with it.

Purificator :
Since no process dynamics are considered for the purificator, the suitable recipe function for the purificator is given by Equation 2.38.

Control problem formulation
The control problem is formulated using the suitable recipe functions given by Equations 3.8 and 3.10 - 3.12, as per the continuous time formulation presented in section 2.1. The objective function remains exactly the same as in section 2.2.1.

Computational result
A maximum profit of 120.0232 MU is achieved over a makespan of 25 hours and the corresponding production schedule is presented in Figure 3.6. The optimal solution was found to converge at 4 event points.

It needs to be mentioned that the control problem solution actually gives a maximum profit of 116.2852 MU. However, this profit is obtained by using just the value of the energy resource Qr, given by Equation 3.10. The true profit value is obtained by replacing this

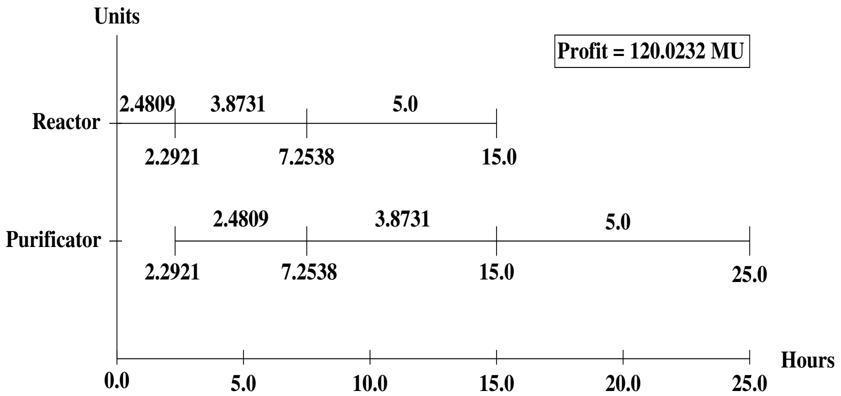

Figure 3.6: Optimal schedule obtained via the IA for example 1.

value with the true Qr for the different batch sizes and their respective processing durations obtained by the control problem solution. The true Qr is evaluated from Equations 2.30 - 2.34. Table 3.5 shows the fitted as well as the true energy resource requirement Qr for the different batch sizes and their respective processing durations shown in Figure 3.6.

Table 3.5: The fitted and the true Qr for the batch sizes shown in Figure 3.6.

vol (m^3)	dur $(hours)$	Qr (fitted) (m^3)	Qr (true) (m^3)
2.4809	2.2921	8.4038	8.3372
3.8731	4.9617	10.8087	10.1497
5.0	7.7462	12.5014	12.2925

Comparison with the solutions obtained via the SRA and the OOA

Table 3.6 shows the model statistics and the solutions obtained via the SRA (using the objective function given by Equation 2.35 in section 2.2.1), the OOA and the IA for this example. As expected, the solution obtained by the OOA is definitely the best. However, as discussed in the previous chapter, this approach is largely inapplicable to the problems of practical size.

The most interesting thing to note in Table 3.6 is that the IA results in a maximum profit that is higher than the SRA with exactly the same model statistics. This increase in the maximum profit is due to an increase in the degrees of freedom. This becomes evident from Figure 3.7, which shows the control profiles followed by the IA and the SBO for a

Table 3.6: Comparison of the SRA, the OOA and the IA results for example 1.

	SRA	OOA	IA
Integer variables	8	8	8
Continuous variables	53	1672	53
Equations	89	1297	89
Solution (MU)	116.1633	122.3952	120.0232

batch size of 2.4809 m^3. Table 3.7 shows the data corresponding to the control profiles shown in Figure 3.7. This data illustrates the ability of the IA to manipulate the control strategies so as to achieve higher overall profit for the plant, instead of confining itself to the control strategies obtained by the SBO.

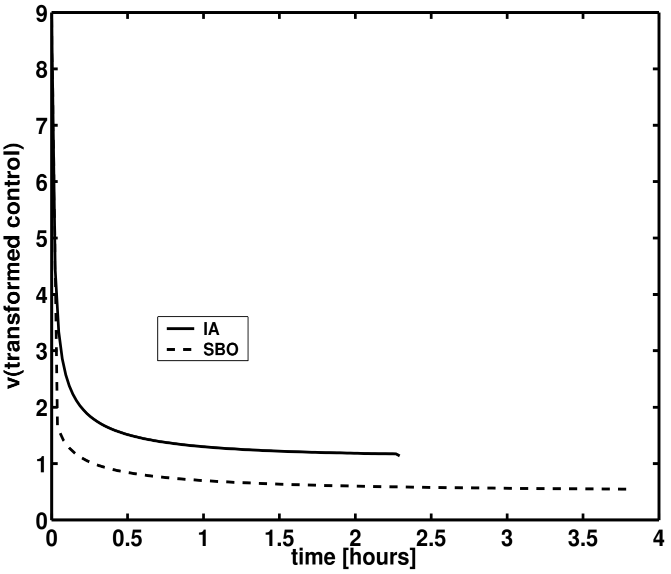

Figure 3.7: Control profiles for the reaction task with batch size 2.4809 m^3 in example 1.

3.2.2 Example 2

The multiple product plant presented in section 2.2.2 is re-considered here. The process flowsheet, the STN representation, the objective of the control problem and all the other data remain exactly the same as in 2.2.2. The control problem formulation for this plant with via the IA is as follows:

Table 3.7: Optimization results for the reaction task with batch size 2.4809 m^3 in example 1.

vol = 2.4809 m^3		
	SBO	IA
$dur\ (hours)$	3.8295	2.2921
$Qr\ (m^3)$	6.7626	8.3372
Cost (MU)	31.6458	36.3657

Determination of suitable recipe functions

Reactors :

The following two SBO problems are solved for each of the reactions on these reactors.

SBO problem 1

The minimum processing durations for different batch sizes and for all the reactions are determined in this approach by solving the following SBO problems :
$\forall k$,

$$minimize \quad dur_0 \tag{3.13}$$

subject to

$$Equations \quad 2.46 - 2.54$$

Table 3.8: Minimum processing durations for different batch sizes for the reactions in example 2.

reaction 1		reaction 2		reaction 3	
vol (m^3)	dur_0 $(hours)$	vol (m^3)	dur_0 $(hours)$	vol (m^3)	dur_0 $(hours)$
0.2	3.8328	0.2	2.7124	0.2	1.7367
0.4	3.8528	0.4	2.7306	0.4	1.7566
⋮	⋮	⋮	⋮	⋮	⋮
2.0	6.6446	2.0	4.6766	2.0	3.0034

Once again, the SBO problems are solved using the standard trapezoidal rule with 100 equidistant time points. The results obtained thereby are presented in Table 3.8 and the corresponding optimal control profiles are shown in Figures 3.8 - 3.13.

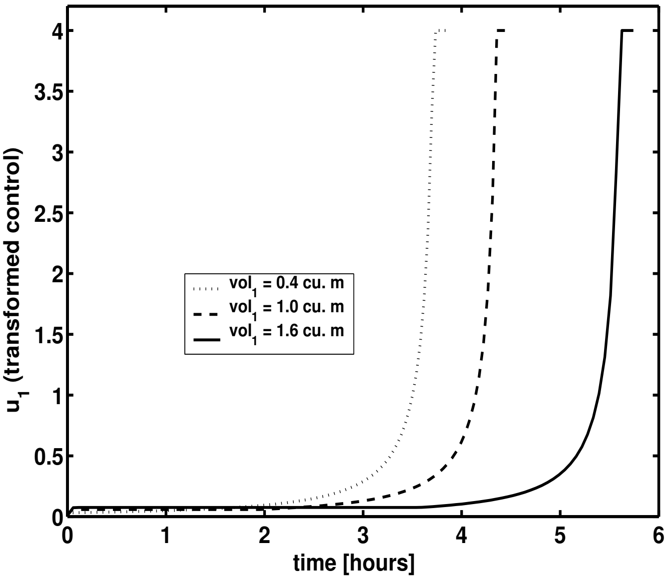

Figure 3.8: Optimal control profiles (u) corresponding to the minimum processing durations for different batch sizes for reaction 1 in example 2.

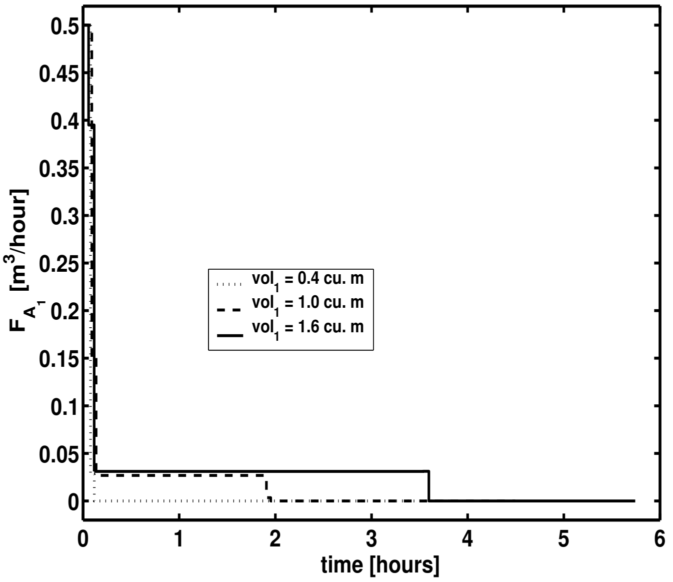

Figure 3.9: Optimal control profiles (F_A) corresponding to the minimum processing durations for different batch sizes for reaction 1 in example 2.

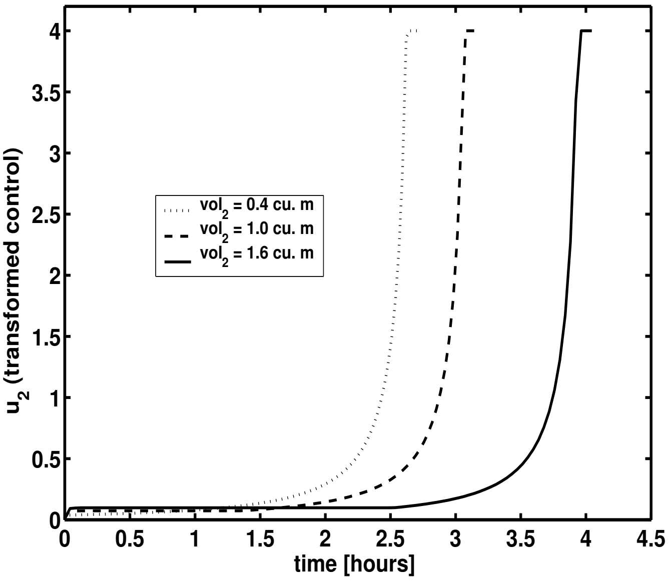

Figure 3.10: Optimal control profiles (u) corresponding to the minimum processing durations for different batch sizes for reaction 2 in example 2.

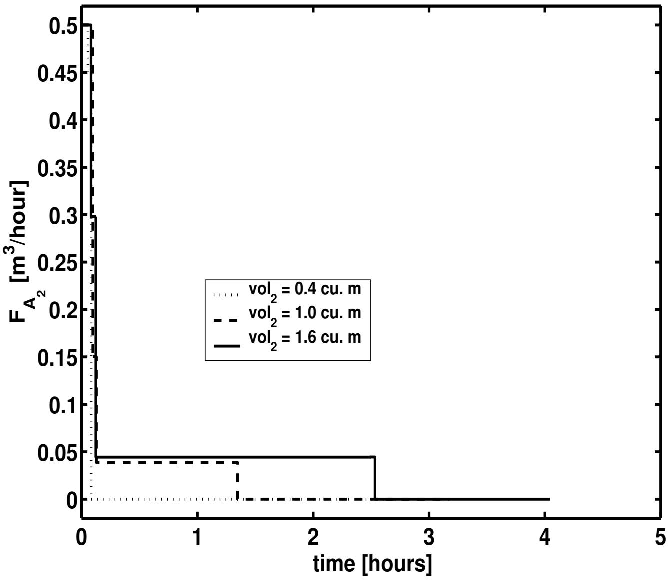

Figure 3.11: Optimal control profiles (F_A) corresponding to the minimum processing durations for different batch sizes for reaction 2 in example 2.

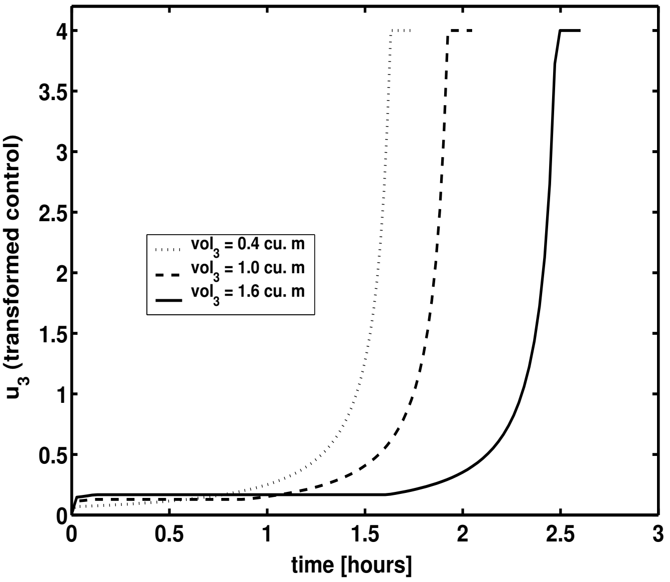

Figure 3.12: Optimal control profiles (u) corresponding to the minimum processing durations for different batch sizes for reaction 3 in example 2.

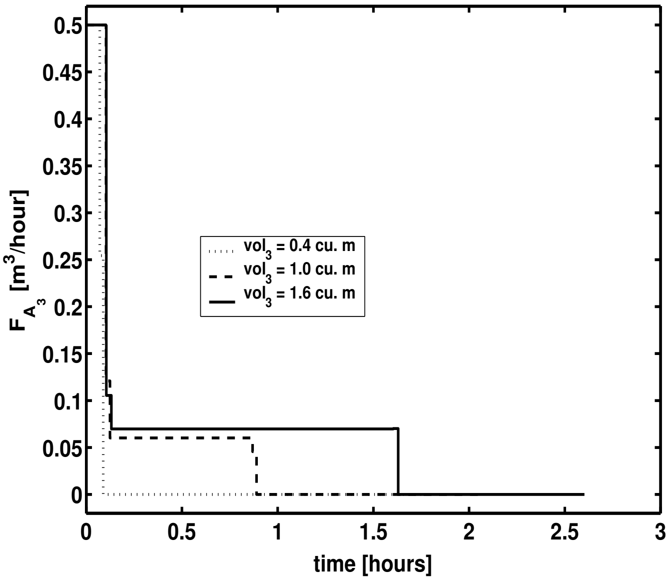

Figure 3.13: Optimal control profiles (F_A) corresponding to the minimum processing durations for different batch sizes for reaction 3 in example 2.

The dependence of the minimum processing duration on the batch size for every reaction is determined via suitable polynomial fitting of the data presented in Table 3.8 and are expressed by Equations 3.14 - 3.19. The corresponding polynomial plots along with their residuals are shown in Figures 3.14 - 3.16.

$$dur_0(1,1,n) = \begin{cases} 0, & vol(1,1,n) = 0 \\ 3.502 + 3.6 \cdot vol(1,1,n) - 13.71 \cdot vol(1,1,n)^2 & \\ +23.3 \cdot vol(1,1,n)^3 - 17.77 \cdot vol(1,1,n)^4 & \\ +6.486 \cdot vol(1,1,n)^5 - 0.9205 \cdot vol(1,1,n)^6, & vol(1,1,n) > 0 \end{cases} \tag{3.14}$$

$$dur_0(2,2,n) = \begin{cases} 0, & vol(2,2,n) = 0 \\ 3.502 + 3.6 \cdot vol(2,2,n) - 13.71 \cdot vol(2,2,n)^2 & \\ +23.3 \cdot vol(2,2,n)^3 - 17.77 \cdot vol(2,2,n)^4 & \\ +6.486 \cdot vol(2,2,n)^5 - 0.9205 \cdot vol(2,2,n)^6, & vol(2,2,n) > 0 \end{cases} \tag{3.15}$$

$$dur_0(3,1,n) = \begin{cases} 0, & vol(3,1,n) = 0 \\ 2.482 + 2.467 \cdot vol(3,1,n) - 9.225 \cdot vol(3,1,n)^2 & \\ +15.53 \cdot vol(3,1,n)^3 - 11.73 \cdot vol(3,1,n)^4 & \\ +4.25 \cdot vol(3,1,n)^5 - 0.5994 \cdot vol(3,1,n)^6, & vol(3,1,n) > 0 \end{cases} \tag{3.16}$$

$$dur_0(4,2,n) = \begin{cases} 0, & vol(4,2,n) = 0 \\ 2.482 + 2.467 \cdot vol(4,2,n) - 9.225 \cdot vol(4,2,n)^2 & \\ +15.53 \cdot vol(4,2,n)^3 - 11.73 \cdot vol(4,2,n)^4 & \\ +4.25 \cdot vol(4,2,n)^5 - 0.5994 \cdot vol(4,2,n)^6, & vol(4,2,n) > 0 \end{cases} \tag{3.17}$$

$$dur_0(5,1,n) = \begin{cases} 0, & vol(5,1,n) = 0 \\ 1.571 + 1.711 \cdot vol(5,1,n) - 6.159 \cdot vol(5,1,n)^2 & \\ +10.24 \cdot vol(5,1,n)^3 - 7.716 \cdot vol(5,1,n)^4 & \\ +2.792 \cdot vol(5,1,n)^5 - 0.3933 \cdot vol(5,1,n)^6, & vol(5,1,n) > 0 \end{cases} \tag{3.18}$$

$$dur_0(6,2,n) = \begin{cases} 0, & vol(6,2,n) = 0 \\ 1.571 + 1.711 \cdot vol(6,2,n) - 6.159 \cdot vol(6,2,n)^2 & \\ +10.24 \cdot vol(6,2,n)^3 - 7.716 \cdot vol(6,2,n)^4 & \\ +2.792 \cdot vol(6,2,n)^5 - 0.3933 \cdot vol(6,2,n)^6, & vol(6,2,n) > 0 \end{cases} \tag{3.19}$$

SBO problem 2

The minimum energy resource Qr required for different batch sizes over different processing durations and for each reaction is determined in this step by solving the following SBO problems. The results obtained thereby are presented in Tables 3.9 - 3.11 and the corresponding optimal control profiles are shown in Figures 3.17 - 3.22. For the sake of brevity, the optimal control profiles are shown only for a single batch size of 1.0 m^3.
$\forall k$

$$minimize \quad Qr \tag{3.20}$$

subject to

$$Equations \ \ 2.46 - 2.54$$

The remaining recipe functions, as given by Equations 3.21 - 3.38, are determined by

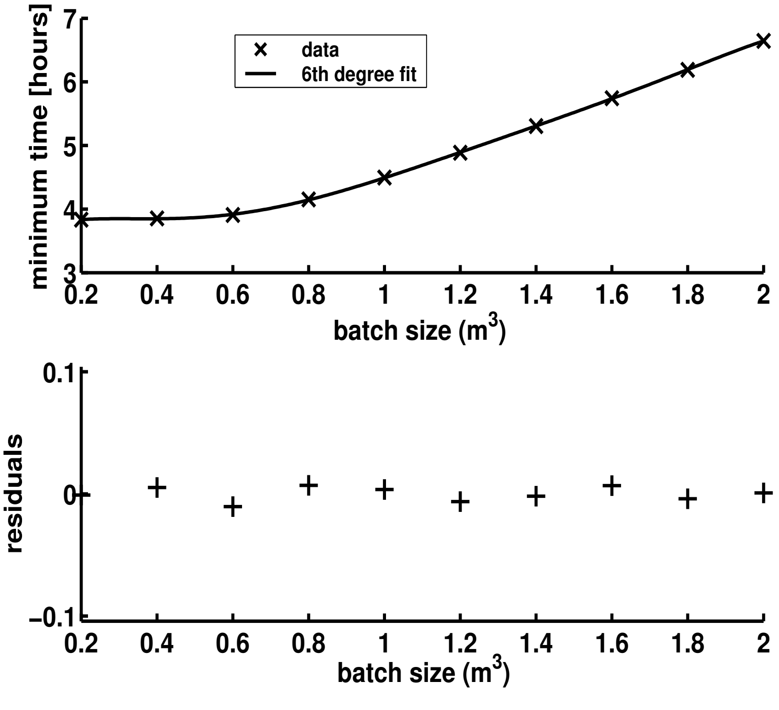

Figure 3.14: Plot of the polynomial given in Equations 3.14 and 3.15.

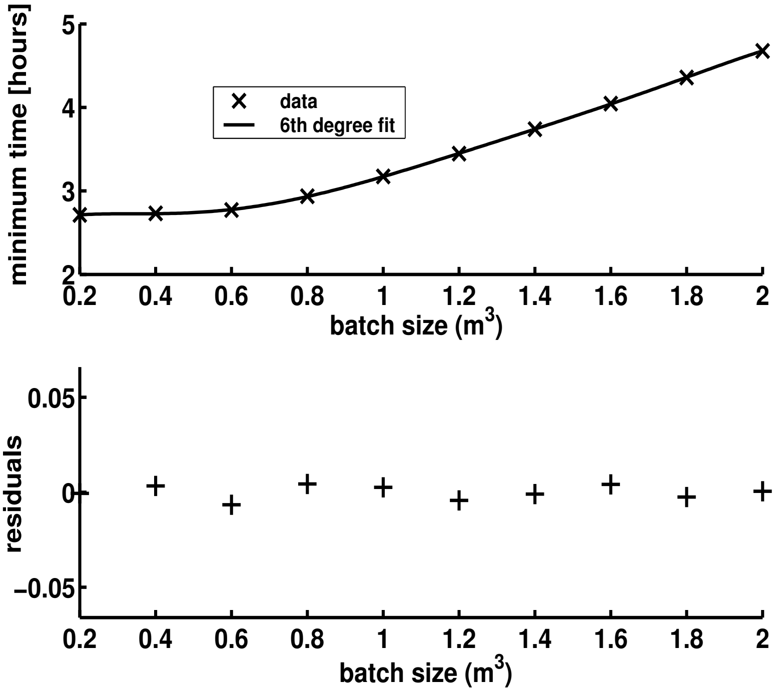

Figure 3.15: Plot of the polynomial given in Equations 3.16 and 3.17.

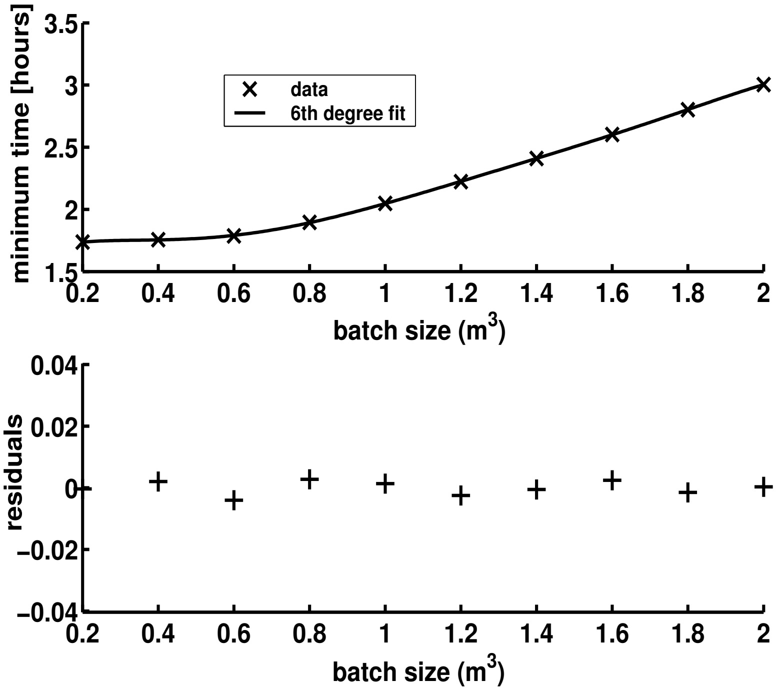

Figure 3.16: Plot of the polynomial given in Equations 3.18 and 3.19.

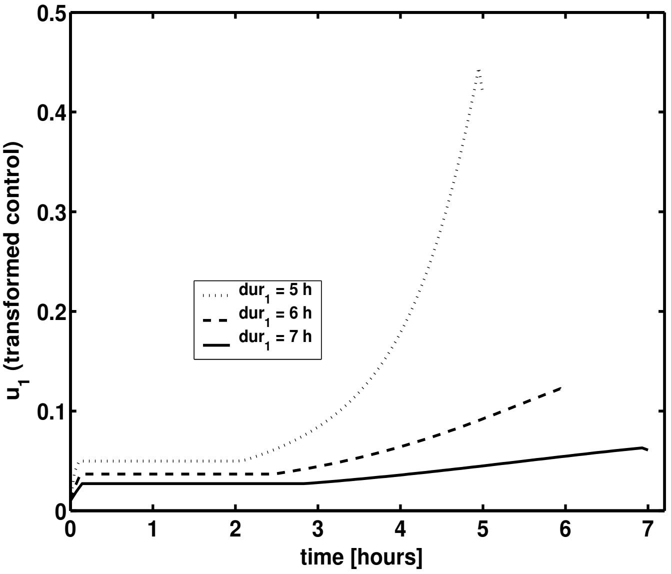

Figure 3.17: Optimal control profiles (u) corresponding to different processing durations for a batch size of 1.0 m^3 and for reaction 1 in example 2.

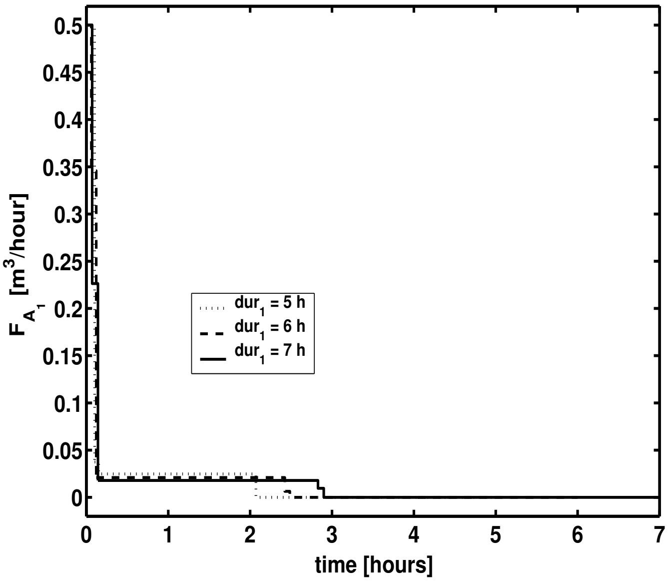

Figure 3.18: Optimal control profiles (F_A) corresponding to different processing durations for a batch size of 1.0 m^3 and for reaction 1 in example 2.

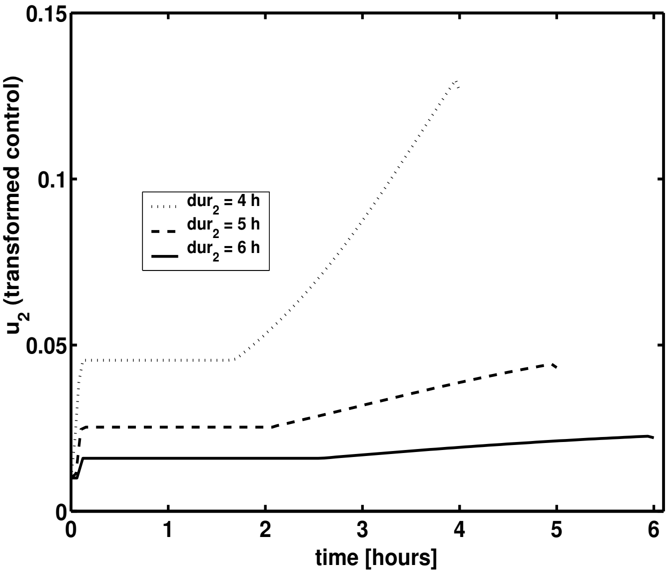

Figure 3.19: Optimal control profiles (u) corresponding to different processing durations for a batch size of 1.0 m^3 and for reaction 2 in example 2.

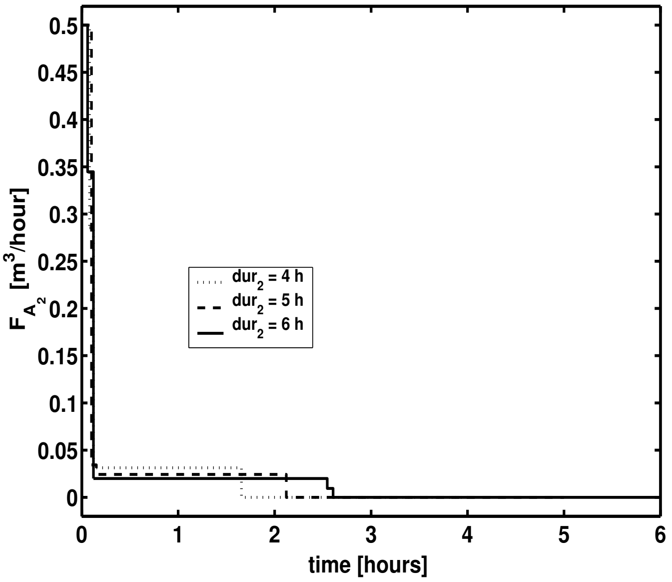

Figure 3.20: Optimal control profiles (F_A) corresponding to different processing durations for a batch size of 1.0 m^3 and for reaction 2 in example 2.

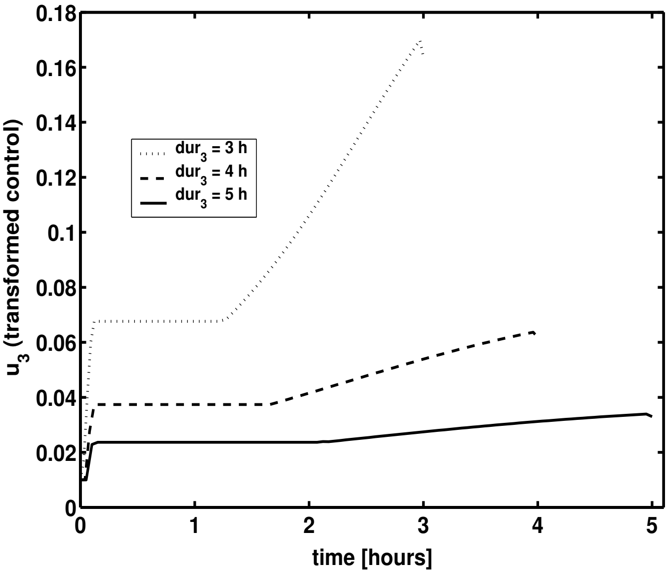

Figure 3.21: Optimal control profiles (u) corresponding to different processing durations for a batch size of 1.0 m^3 and for reaction 3 in example 2.

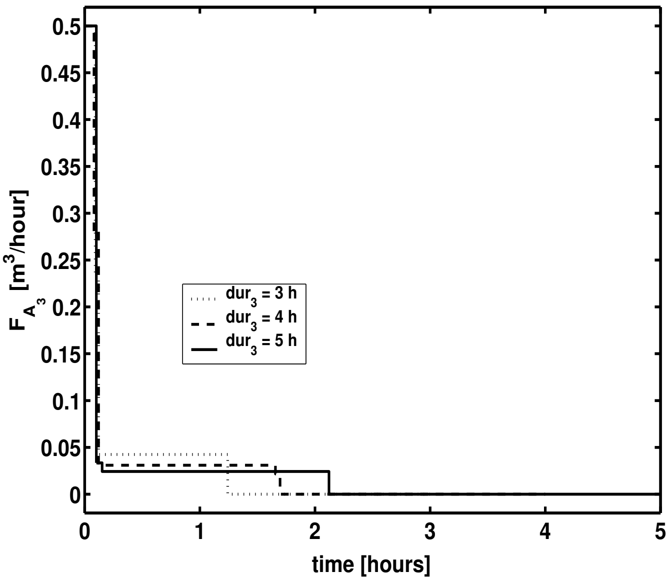

Figure 3.22: Optimal control profiles (F_A) corresponding to different processing durations for a batch size of 1.0 m^3 and for reaction 3 in example 2.

Table 3.9: Data corresponding to the optimal control profiles for different batch sizes and for the reaction 1 in example 2.

0.2 m^3		0.4 m^3		…	2.0 m^3	
dur $(hours)$	Qr	dur $(hours)$	Qr	… …	dur $(hours)$	Qr
3.8328	1.4871	3.8528	1.4877	…	6.6446	1.7930
4.25	0.5746	4.25	0.5869	…	6.75	1.20
4.5	0.4669	4.5	0.4740	…	7.0	0.8942
⋮	⋮	⋮	⋮	…		
7.0	0.1885	7.0	0.1889	…		

Table 3.10: Data corresponding to the optimal control profiles for different batch sizes and for the reaction 2 in example 2.

0.2 m^3		0.4 m^3		…	2.0 m^3	
dur $(hours)$	Qr	dur $(hours)$	Qr	… …	dur $(hours)$	Qr
2.7124	1.2332	2.7306	1.2334	…	4.6766	1.5046
3.0	0.4183	3.0	0.4327	…	5.0	0.6486
3.25	0.2993	3.25	0.3063	…	5.25	0.5282
⋮	⋮	⋮	⋮	…	⋮	⋮
7.0	0.0700	7.0	0.0700	…	7.0	0.2644

using the data presented in Tables 3.9 - 3.11.

$$Qr(1,1,n) = \begin{cases} 0, & vol(1,1,n) = 0 \\ (24.1268 + 5.9706 \cdot vol(1,1,n) & \\ -12.0213 \cdot dur(1,1,n) + 6.2806 \cdot vol(1,1,n)^2 & \\ -3.2029 \cdot vol(1,1,n) \cdot dur(1,1,n) & \\ +2.0583 \cdot dur(1,1,n)^2 - 0.9790 \cdot vol(1,1,n)^3 & \\ -1.3104 \cdot vol(1,1,n)^2 \cdot dur(1,1,n) & \\ +0.3882 \cdot vol(1,1,n) \cdot dur(1,1,n)^2 & \\ -0.1197 \cdot dur(1,1,n)^3), & vol(1,1,n) > 0 \end{cases} \tag{3.21}$$

$$dur(1,1,n) = 0, \quad \forall\, vol(1,1,n) = 0 \tag{3.22}$$

Table 3.11: Data corresponding to the optimal control profiles for different batch sizes and for the reaction 3 in example 2.

0.2 m^3		0.4 m^3		$\ldots$	2.0 m^3	
dur $(hours)$	Qr	dur $(hours)$	Qr	$\ldots$ $\ldots$	dur $(hours)$	Qr
1.7367	1.1880	1.7566	1.1899	$\ldots$	3.0034	1.4795
2.0	0.4750	2.0	0.4924	$\ldots$	3.25	0.7654
2.25	0.3448	2.25	0.3529	$\ldots$	3.5	0.6111
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\ldots$	$\vdots$	$\vdots$
7.0	0.0700	7.0	0.0700	$\ldots$	7.0	0.2198

$$dur(1,1,n) \geq dur_0(1,1,n) \ + \ \delta(1,1,n), \quad \forall \, vol(1,1,n) > 0 \tag{3.23}$$

$$Qr(2,2,n) = \begin{cases} 0, & vol(2,2,n) = 0 \\ (24.1268 + 5.9706 \cdot vol(2,2,n) & \\ -12.0213 \cdot dur(2,2,n) + 6.2806 \cdot vol(2,2,n)^2 & \\ -3.2029 \cdot vol(2,2,n) \cdot dur(2,2,n) & \\ +2.0583 \cdot dur(2,2,n)^2 - 0.9790 \cdot vol(2,2,n)^3 & \\ -1.3104 \cdot vol(2,2,n)^2 \cdot dur(2,2,n) & \\ +0.3882 \cdot vol(2,2,n) \cdot dur(2,2,n)^2 & \\ -0.1197 \cdot dur(2,2,n)^3), & vol(2,2,n) > 0 \end{cases} \tag{3.24}$$

$$dur(2,2,n) = 0, \quad \forall \, vol(2,2,n) = 0 \tag{3.25}$$

$$dur(2,2,n) \geq dur_0(2,2,n) \ + \ \delta(2,2,n), \quad \forall \, vol(2,2,n) > 0 \tag{3.26}$$

$$Qr(3,1,n) = \begin{cases} 0, & vol(3,1,n) = 0 \\ (8.7174 + 2.4525 \cdot vol(3,1,n) & \\ -4.8829 \cdot dur(3,1,n) + 2.2293 \cdot vol(3,1,n)^2 & \\ -1.5309 \cdot vol(3,1,n) \cdot dur(3,1,n) & \\ +0.9552 \cdot dur(3,1,n)^2 + 0.1079 \cdot vol(3,1,n)^3 & \\ -0.3878 \cdot vol(3,1,n)^2 \cdot dur(3,1,n) & \\ +0.1829 \cdot vol(3,1,n) \cdot dur(3,1,n)^2 & \\ -0.0624 \cdot dur(3,1,n)^3), & vol(3,1,n) > 0 \end{cases} \tag{3.27}$$

$$dur(3,1,n) = 0, \quad \forall \, vol(3,1,n) = 0 \tag{3.28}$$

$$dur(3,1,n) \geq dur_0(3,1,n) \ + \ \delta(3,1,n), \quad \forall\, vol(3,1,n) > 0 \tag{3.29}$$

$$Qr(4,2,n) = \begin{cases} 0, & vol(4,2,n) = 0 \\ (8.7174 + 2.4525 \cdot vol(4,2,n) & \\ -4.8829 \cdot dur(4,2,n) + 2.2293 \cdot vol(4,2,n)^2 & \\ -1.5309 \cdot vol(4,2,n) \cdot dur(4,2,n) & \\ +0.9552 \cdot dur(4,2,n)^2 + 0.1079 \cdot vol(4,2,n)^3 & \\ -0.3878 \cdot vol(4,2,n)^2 \cdot dur(4,2,n) & \\ +0.1829 \cdot vol(4,2,n) \cdot dur(4,2,n)^2 & \\ -0.0624 \cdot dur(4,2,n)^3), & vol(4,2,n) > 0 \end{cases} \tag{3.30}$$

$$dur(4,2,n) = 0, \quad \forall\, vol(4,2,n) = 0 \tag{3.31}$$

$$dur(4,2,n) \geq dur_0(4,2,n) \ + \ \delta(4,2,n), \quad \forall\, vol(4,2,n) > 0 \tag{3.32}$$

$$Qr(5,1,n) = \begin{cases} 0, & vol(5,1,n) = 0 \\ (3.8960 + 1.1574 \cdot vol(5,1,n) & \\ -2.3643 \cdot dur(5,1,n) - 0.0378 \cdot vol(5,1,n)^2 & \\ -0.3721 \cdot vol(5,1,n) \cdot dur(5,1,n) & \\ +0.4769 \cdot dur(5,1,n)^2 + 0.2830 \cdot vol(5,1,n)^3 & \\ -0.1478 \cdot vol(5,1,n)^2 \cdot dur(5,1,n) & \\ +0.0536 \cdot vol(5,1,n) \cdot dur(5,1,n)^2 & \\ -0.0316 \cdot dur(5,1,n)^3), & vol(5,1,n) > 0 \end{cases} \tag{3.33}$$

$$dur(5,1,n) = 0, \quad \forall\, vol(5,1,n) = 0 \tag{3.34}$$

$$dur(5,1,n) \geq dur_0(5,1,n) \ + \ \delta(5,1,n), \quad \forall\, vol(5,1,n) > 0 \tag{3.35}$$

$$Qr(6,2,n) = \begin{cases} 0, & vol(6,2,n) = 0 \\ (3.8960 + 1.1574 \cdot vol(6,2,n) & \\ -2.3643 \cdot dur(6,2,n) - 0.0378 \cdot vol(6,2,n)^2 & \\ -0.3721 \cdot vol(6,2,n) \cdot dur(6,2,n) & \\ +0.4769 \cdot dur(6,2,n)^2 + 0.2830 \cdot vol(6,2,n)^3 & \\ -0.1478 \cdot vol(6,2,n)^2 \cdot dur(6,2,n) & \\ +0.0536 \cdot vol(6,2,n) \cdot dur(6,2,n)^2 & \\ -0.0316 \cdot dur(6,2,n)^3), & vol(6,2,n) > 0 \end{cases} \tag{3.36}$$

$$dur(6,2,n) = 0, \quad \forall\, vol(6,2,n) = 0 \tag{3.37}$$

$$dur(6,2,n) \geq dur_0(6,2,n) \ + \ \delta(6,2,n), \quad \forall\, vol(6,2,n) > 0 \tag{3.38}$$

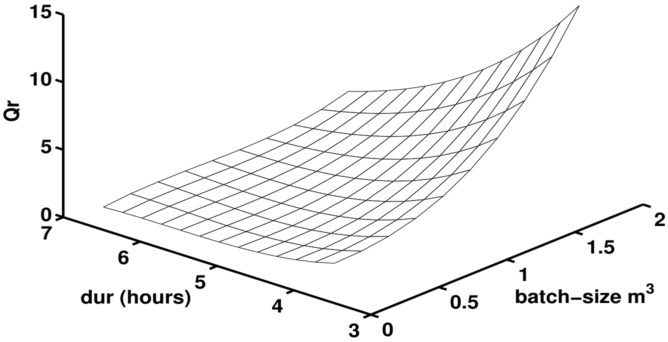

Figure 3.23: Plot of the third order polynomial given in Equations 3.21 and 3.24.

where, the values for $\delta(i, j, n)$ in the Equations 3.21 - 3.38 correspond to the largest residuals below zero in the Figures 3.14 - 3.16 and are given as follows:

$$\delta(1, 1, n) = \delta(2, 2, n) = 0.0106$$
$$\delta(3, 1, n) = \delta(4, 2, n) = 0.0066$$
$$\delta(5, 1, n) = \delta(6, 2, n) = 0.0041$$

Equations 3.21, 3.24, 3.27, 3.30, 3.33 and 3.36 are obtained via third order polynomial regression of the data presented in Tables 3.9 - 3.11 and the corresponding polynomial plots are presented in Figures 3.23 - 3.25. It is clear from these figures that the obtained polynomials are very smooth and thus, computation friendly.

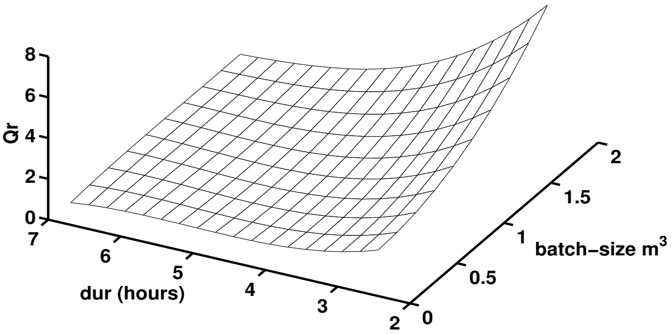

Figure 3.24: Plot of the third order polynomial given in Equations 3.27 and 3.30.

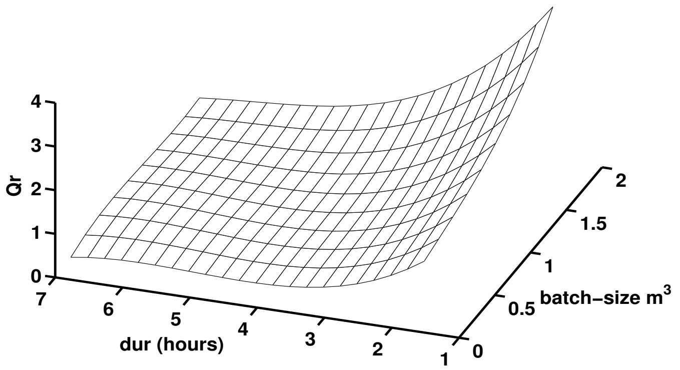

Figure 3.25: Plot of the third order polynomial given in Equations 3.33 and 3.36.

Purificators :
The suitable recipe functions for the purificators remain unchanged and are given by Equations 2.57 - 2.59.

Control problem formulation
The control problem is formulated using the suitable recipe functions given by the Equations 3.14 - 3.19 and 3.21 - 3.38. The objective function and the control problem formulation remain exactly the same as in section 2.2.2.

Computational result
A maximum profit of 38.3502 MU is achieved over a makespan of 7.0 hours and the corresponding production schedule is shown in Figure 3.26. The optimal solution was found to converge at five event points.

Here 38.3502 MU is the true profit value, which is obtained by replacing the fitted energy resource requirement Qr with the true Qr for the different batch sizes and their respective processing durations obtained by the control problem solution. The fitted as well as the true energy resource requirement Qr for the different batch sizes and their respective processing durations shown in Figure 3.26 are presented in Table 3.12.

Comparison with the solutions obtained via the SRA and the OOA
The model statistics and the solutions obtained via the SRA, the OOA and the IA for this example are presented in Table 3.13. The maximum profit obtained with the IA is significantly higher than that obtained with the SRA with exactly the same model

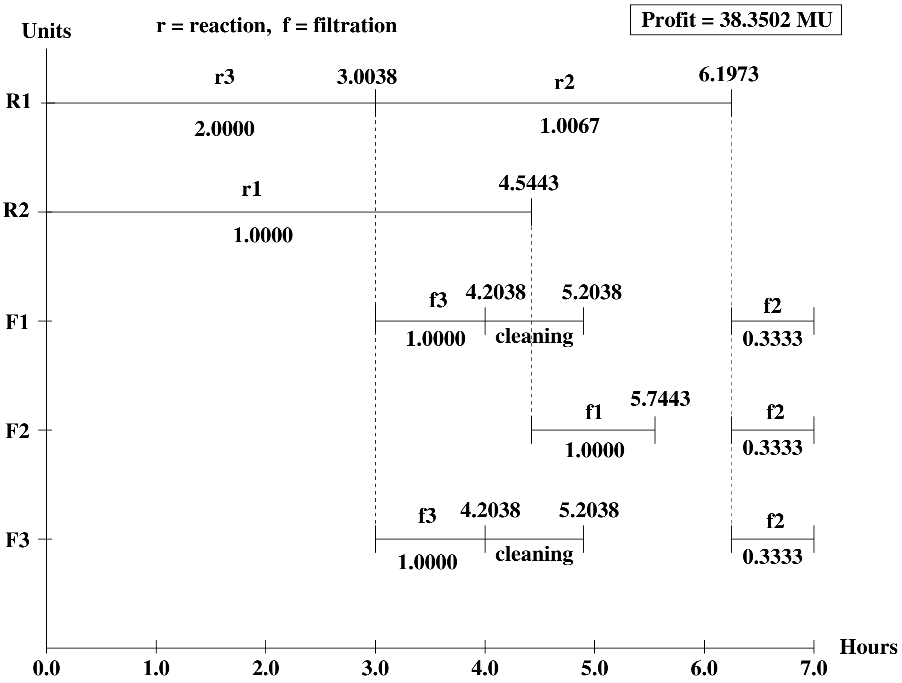

Figure 3.26: Optimal schedule obtained via the IA for example 2.

statistics and nearly the same CPU timing. This is again due to more degrees of freedom in the IA control problem than the SRA control problem, as discussed in section 3.2.1.

Interestingly, the IA solution for this example is better than the OOA solution as well. This is because the IA control problem could be solved with 5 event points in acceptable computation time, which was not possible for the OOA control problem. The OOA control problem for this example, as mentioned earlier, could be solved only with a maximum of 4 event points and for that too, it needed a CPU timing that was nearly 29 times higher than that needed by the SRA and the IA control problems for this example. However, here

Table 3.12: The fitted and the true Qr for the batch sizes shown in Figure 3.26.

vol (m^3)	dur ($hours$)	Qr (fitted)	Qr (true)
1.0000 (reaction 1)	4.5443	1.5077	1.1303
1.0067 (reaction 2)	3.1935	1.3723	1.0614
2.0000 (reaction 3)	3.0038	1.6242	1.4424
1.0000 (reaction 3)	2.0557	1.3369	1.0893

it needs to be pointed out that the CPU timings for the SRA and the IA presented in Table 3.13 do not include the significant amount of time needed for determining the recipes or the suitable recipe functions.

Table 3.13: Comparison of the SRA, the OOA and the IA results for example 2.

	SRA (5 event points)	OOA (4 event points)	IA (5 event points)
Integer variables	75	60	75
Continuous variables	441	12969	441
Equations	1143	9864	1143
Solution (MU)	31.9093	36.5287	38.3502
CPU time(s)	99.53	2885.85	99.71

For the sake of true comparison of the performance of the IA and the OOA, the IA control problem for this example was also solved with 4 event points. A maximum profit of 36.3889 MU is obtained with 4 event points, which is in very close agreement with the solution obtained via the OOA with the same number of event points. This indicates that the IA control problem is nearly as good as the OOA control problem as far as the number of degrees of freedom are concerned. However, in terms of computational requirements, the IA is far superior to the OOA, as shown in Table 3.13.

3.3 Summary

In this chapter, an improved approach (IA) is proposed for the control of MBPs. The proposed approach is applied to illustrative examples and the results obtained thereby are compared to that obtained via the SRA and the OOA for these examples.

The results presented in this chapter, particularly in section 3.2.2, highlight the fact that the IA control problems indeed possess the computational features like the SRA control problems. However, the degrees of freedom possessed by them is higher than the SRA control problems. It can be conveniently concluded that just like the OOA, the solutions obtained via the IA also would be ”at least” as good as the SRA, if not better.

The results obtained for the illustrative examples clearly advocate that the IA is probably the most suitable approach for the control of MBPs and can be applied to the real world problems due to its computational features. This is further investigated with the help of a detailed application example in the next chapter.

Chapter 4

An Application Example

In this chapter, the improved approach for the control of MBPs is applied to a more realistic example with detailed process dynamics.

The plant considered here comprises of two non-isothermal batch reactors (R1 and R2) and a set of three batch purificators (P1, P2 and P3), as shown in Figure 4.1. Once again, the zero-wait policy is assumed for the operation of the plant. Two different products (B1 and B2) are to be produced in this plant from two different reactants (A1 and A2) and the

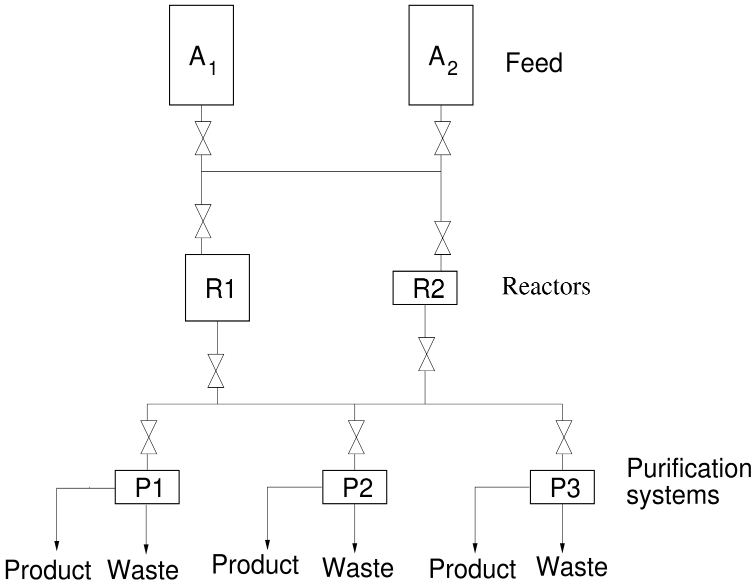

Figure 4.1: Flow sheet of the application example.

processing stages involved are described in the following:

Reactors :

The reactors in the plant are assumed to be non-isothermal batch reactors, as shown in Figure 4.2, with the following exothermic series reactions to be executed:

$$A_x \longrightarrow B_x \longrightarrow C_x \quad ; \qquad x = 1, 2$$
$$A_x = \text{reactant}, B_x = \text{desired product}, C_x = \text{by-product}$$

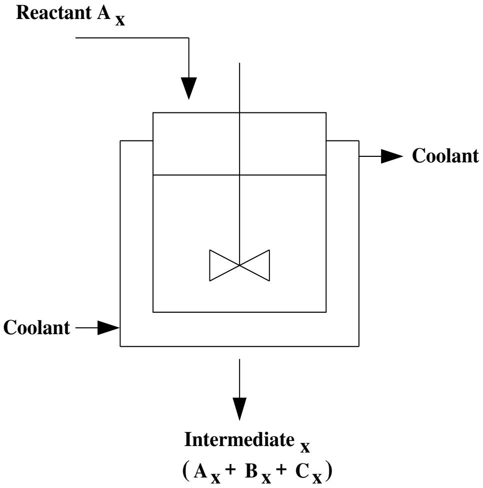

Figure 4.2: A schematic of the batch reactors in the application example.

Before every reaction, the reactors are filled with the desired amount of reactant and then the reaction is carried out until a desired concentration of the product is reached, while keeping a check on the amount of by-product produced during the reaction. The optimal temperature profile in the reactor is maintained by appropriately regulating the coolant flow rate into the reactor jacket. Assuming perfect mixing inside the reactors, the governing equations for the these reactors are given as follows:

Material balances inside the reactor

$$\frac{dC_{A_x}(t)}{dt} = -k_{1_x} \cdot C_{A_x}(t) \tag{4.1}$$

$$\frac{dC_{B_x}(t)}{dt} = k_{1_x} \cdot C_{A_x}(t) - k_{2_x} \cdot C_{B_x}(t) \tag{4.2}$$

$$\frac{dC_{C_x}(t)}{dt} = k_{2_x} \cdot C_{B_x}(t) \tag{4.3}$$

Energy balance inside the reactor

$$\frac{dT_x(t)}{dt} = \frac{Q_{r_x} - Q_{m_x}}{C_{p_x} \cdot V_x \cdot \rho_x} \tag{4.4}$$

Energy balance for the reactor wall

$$\frac{dT_{m_x}(t)}{dt} = \frac{Q_{m_x} - Q_J}{C_{pm} \cdot V_{m_r} \cdot \rho_m} \tag{4.5}$$

Energy balance for the reactor jacket

$$\frac{dT_{J_x}(t)}{dt} = \frac{F_{J_x}(t)}{V_{J_r}} \cdot (T_{J0} - T_{J_x}(t)) + \frac{Q_{J_x}}{C_{pJ} \cdot V_{J_r} \cdot \rho_J} \tag{4.6}$$

Heat of reaction

$$Q_{r_x} = -\Delta H_{1_x} \cdot (k_{1_x} \cdot C_{A_x}(t) \cdot V_x) - \Delta H_{2_x} \cdot (k_{2_x} \cdot C_{B_x}(t) \cdot V_x) \tag{4.7}$$

Heat transfer due to the coolant

$$Q_{m_x} = U_i \cdot A_{i_r} \cdot (T_x(t) - T_{m_x}(t)) \tag{4.8}$$

$$Q_{J_x} = U_o \cdot A_{o_r} \cdot (T_{m_x}(t) - T_{J_x}(t)) \tag{4.9}$$

Reaction kinetics

$$k_{1_x} = k_{10_x} \cdot exp\left(- \frac{E_{1_x}}{R \cdot T_x(t)} \right) \tag{4.10}$$

$$k_{2_x} = k_{20_x} \cdot exp\left(- \frac{E_{2_x}}{R \cdot T_x(t)} \right) \tag{4.11}$$

$$T_x(t) \ \leq \ T_{up_x} \tag{4.12}$$

$$T_x(t = dur_x) \ = \ T_{sat_x} \tag{4.13}$$

$$C_{C_x}(t = dur_x) \ \leq \ C_{C_{max_x}} \tag{4.14}$$

$$C_{B_x}(t = dur_x) \; = \; C_{B_{int_x}} \tag{4.15}$$

$$coolant_x = \int_0^{dur_x} F_{J_x}(t) \cdot dt \tag{4.16}$$

where, $t \in [0,\ dur]$ and the notations have the following meaning:

A_{i_r} ... inner surface area of reactor r, where $r \in \{1, 2\}$

A_{o_r} ... outer surface area of reactor r

$C_{i_x}(t)$ ... concentration of component i in reaction x at time t

C_{p_x} ... specific heat of the reactant in reaction x

C_{pm} ... specific heat of the reactor/purificator metal

C_{pJ} ... specific heat of the coolant/hot water

E_{1_x} ... activation energy 1 for reaction x

E_{2_x} ... activation energy 2 for reaction x

$F_{J_x}(t)$ ... coolant flow rate at time t for reaction x

ΔH_{1_x} ... enthalpy of reaction 1 for reaction x

ΔH_{2_x} ... enthalpy of reaction 2 for reaction x

k_{1_x} ... reaction rate constant 1 for reaction x

k_{2_x} ... reaction rate constant 2 for reaction x

k_{10} ... frequency factor 1 for reaction x

k_{20} ... frequency factor 2 for reaction x

Q_{r_x} ... heat generated during reaction x

Q_{J_x} ... amount of heat transferred to the coolant in reaction x

Q_{m_x} ... amount of heat transferred to the reactor metal in reaction x

R ... universal gas constant

$T_x(t)$ ... temperature of the reaction mixture at time t in reaction x

$T_{J_x}(t)$ ... temperature of coolant at time t in reaction x

T_{J0} ... inlet temperature of coolant

$T_{m_x}(t)$ ... temperature of the reactor metal at time t in reaction x

U_i ... inside heat transfer coefficient of the reactor/purificator metal

U_o ... outside heat transfer coefficient of the reactor/purificator metal

V_x ... volume of the reactor contents in reaction x

V_{J_r} ... volume of the jacket of reactor r

V_{m_r} ... volume of the reactor metal of reactor r

ρ_x ... density of the reacting mixture in reaction x

ρ_m ... density of the reactor/purificator metal

ρ_J … density of the coolant/hot water
$coolant_x$ … total amount of coolant needed for reaction x
T_{up_x} … upper bound on the temperature of the reacting mixture during reaction x
T_{sat_x} … saturation temperature of the intermediate produced from reaction x
$C_{A_x}(t)$ … concentration of reactant A at time t in reaction x
$C_{B_x}(t)$ … concentration of product B at time t in reaction x
$C_{C_x}(t)$ … concentration of by-product C at time t in reaction x
$C_{C_{max_x}}$ … upper limit on the amount of by-product produced during reaction x
$C_{B_{int_x}}$ … final concentration of the desired product B in the intermediate produced from reaction x

Equations 4.1 - 4.11 represent the dynamic mass and energy balances, while Equation 4.12 imposes an upper bound on the temperature of the reactor contents during the process. Equation 4.13 ensures that the intermediates leave the reactors at their respective saturation temperatures. Equation 4.14 imposes an upper bound on the amount of by-product C produced during the reaction, whereas Equation 4.15 ensures that the intermediates leave the reactors with the desired concentration of product B in them.

Table 4.1: Data used for the reactors in the application example.

ΔH_{1_1} = -6.50E8 $J/kmol$	ΔH_{2_1} = -1.20E8 $J/kmol$	ρ_1 = 800.0 kg/m^3
ΔH_{1_2} = -6.80E8 $J/kmol$	ΔH_{2_2} = -1.40E8 $J/kmol$	ρ_2 = 850.0 kg/m^3
ρ_m = 8200.0 kg/m^3	ρ_J = 1000.0 kg/m^3	C_{p_1} = 4200.0 $J/kg\ K$
C_{p_2} = 4600.0 $J/kg\ K$	E_{1_2} = 3.37E7 $J/kmol$	E_{2_2} = 4.29E7 $J/kmol$
C_{pm} = 500.0 $J/kg\ K$	C_{pJ} = 4200.0 $J/kg\ K$	E_{1_1} = 3.49E7 $J/kmol$
E_{2_1} = 4.65E7 $J/kmol$	V_{m_1} = 0.032 m^3	V_{m_2} = 0.02 m^3
V_{J_1} = 0.53 m^3	k_{10_1} = 4.38E4 h^{-1}	k_{20_1} = 3.94E5h^{-1}
V_{J_2} = 0.302 m^3	k_{10_2} = 3.98E4 h^{-1}	k_{20_2} = 4.67E5h^{-1}
R = 8314.0 $J/kmol\ K$	U_i = 7.0E6 $J/h\ K\ m^2$	U_o = 8.18E6 $J/h\ K\ m^2$
A_{i_1} = 5.25 m^2	A_{o_1} = 5.25 m^2	T_{j0} = 298.0 K
A_{i_2} = 3.3 m^2	A_{o_2} = 3.3 m^2	$F_{J_x}(t) \in$ [0.0, 9.0] m^3/h
$T_x(t=0)$ = 350.0 K	$T_{m_x}(t=0)$ = 373.0 K	$T_{J_x}(t=0)$ = 300.0 K
$C_{A_x}(t=0)$ = 0.975 $kmol/m^3$	$C_{B_x}(t=0)$ = 0.025 $kmol/m^3$	$C_{C_x}(t=0)$ = 0.0
T_{up_x} = 370.0 K	T_{sat_1} = 323.0 K	T_{sat_2} = 328.0 K
$C_{C_{max_x}}$ = 0.1 $kmol/m^3$	$C_{B_{int_1}}$ = 0.6 $kmol/m^3$	$C_{B_{int_2}}$ = 0.46 $kmol/m^3$

Finally, Equation 4.16 represents the total amount of coolant utilized during the reaction. It is assumed that the minimum batch size required to start operating the reactors is 0.4 m^3 and 0.2 m^3 for reactors R1 and R2 respectively. The data used for the reactors is given in Table 4.1.

Purificators :

The purificators in the plant are assumed to be non-isothermal batch purificators, as shown in Figure 4.3.

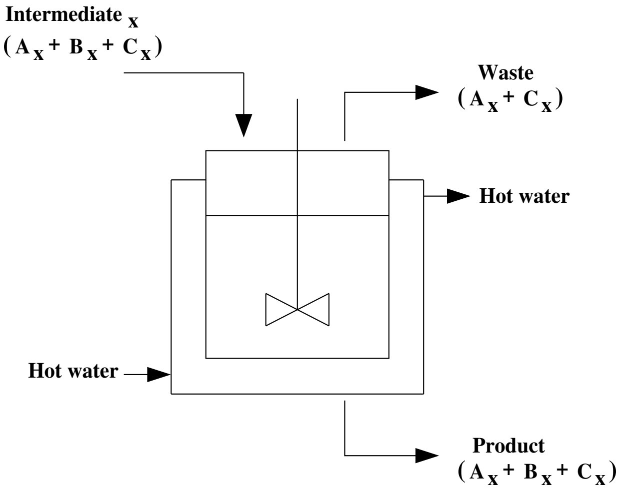

Figure 4.3: A schematic of the batch purificators in the application example.

The intermediates leave the reactors at their respective saturation temperatures and go directly to the purificators, where they are evaporated until a desired concentration of the desired product is reached. It is assumed that the vapor is drawn continuously out of the purifiactor and comprises only of the unreacted reactant and the by-product. It is also assumed that absolutely no amount of the desired product, which is the heavy boiling component, is lost during the process. Under the assumption of perfect mixing inside the purificators, the governing equations for these purificators can be expressed as follows:

Overall material balance inside the purificator

$$\rho_x \cdot \frac{dV_{xp}(t)}{dt} = -M_{v_{xp}} \tag{4.17}$$

Overall energy balance inside the purificator

$$\frac{dH_{xp}(t)}{dt} = -U_i \cdot A_i \cdot (T_{m_{xp}}(t) - T_{sat_x}) - M_{v_{xp}} \cdot H_{v_{xp}} \tag{4.18}$$

Here we make the following simplifying assumptions:

1. The enthalpy of vapor ($H_{v_{xp}}$) is the same as the latent heat of vaporization (H_{latent_x}).
2. The energy balance inside the purificators is assumed to be quasi-static, that is, $\frac{dH_{xp}(t)}{dt} = 0$

With these assumptions, the governing equations for these purificators can be written as follows:

Energy balance for the purificator jacket

$$\frac{dT_{J_{xp}}(t)}{dt} = \frac{F_{J_{xp}}(t)}{V_J} \cdot (T_{J_{in}} - T_{J_{xp}}(t)) - \frac{U_o \cdot A_o \cdot (T_{J_{xp}}(t) - T_{m_{xp}}(t))}{C_{pJ} \cdot V_J \cdot \rho_J} \tag{4.19}$$

Energy balance for the purificator wall (metal)

$$\frac{dT_{m_{xp}}(t)}{dt} = \frac{(U_o \cdot A_o \cdot (T_{J_{xp}} - T_{m_{xp}})) - (U_i \cdot A_i \cdot (T_{m_{xp}}(t) - T_{sat_x}))}{C_{pm} \cdot V_m \cdot \rho_m} \tag{4.20}$$

Overall material balance inside the purificator

$$\frac{dV_{xp}(t)}{dt} = \frac{-U_i \cdot A_i \cdot (T_{m_{xp}}(t) - T_{sat_x})}{\rho_x \cdot H_{latent_x}} \tag{4.21}$$

Material balance for product B_x inside the purificator

$$\frac{dC_{B_{xp}}(t)}{dt} = \frac{U_i \cdot A_i \cdot (T_{m_{xp}}(t) - T_{sat_{xp}}) \cdot C_{B_{xp}}(t)}{\rho_x \cdot V_{xp}(t) \cdot H_{latent_x}} \tag{4.22}$$

Material balance for product B_x at the end of the purification

$$V_{xp}(t = dur_{xp}) = \frac{V_{0_{xp}} \cdot C_{B_{0_{xp}}}}{C_{B_{f_{xp}}}} \tag{4.23}$$

The total amount of hot water utilized during the purification

$$hot\ water_{xp} = \int_0^{dur_{xp}} F_{J_{xp}}(t) \cdot dt \tag{4.24}$$

where, $t \in [0,\ dur]$ and the notations have the following meaning:

A_i ... inner surface area of the purificators
A_o ... outer surface area of the purificators
$T_{J_{xp}}(t)$ ... temperature of hot water at time t while purifying the intermediate produced

from reaction x

$T_{J_{in}}$ ... inlet temperature of hot water

$T_{m_{xp}}(t)$ ... temperature of the purificator metal (wall) at time t while purifying the intermediate produced from reaction x

$V_{xp}(t)$ ... volume of the purificator content at time t while purifying the intermediate produced from reaction x

$V_{0_{xp}}$ ... initial volume of the purificator content while purifying the intermediate produced from reaction x

$M_{v_{xp}}$ ... mass flowrate of vapor while purifying the intermediate produced from reaction x

$H_{v_{xp}}$ ... enthalpy of the vapor leaving the purificator while purifying the intermediate produced from reaction x

$H_{xp}(t)$ ... enthalpy of the intermediate produced from reaction x at time t during purification

V_J ... volume of the jacket of the purificator

V_m ... volume of the purificator metal

H_{latent_x} ... latent heat of the intermediate produced from reaction x

$F_{J_{xp}}(t)$ ... hot water flow rate at time t while purifying the intermediate produced from reaction x

$C_{B_{xp}}(t)$ ... concentration of product B at time t while purifying the intermediate produced from reaction x

$C_{B_{0_{xp}}}$ ... initial concentration of product B while purifying the intermediate produced from reaction x, note that $C_{B_{0_{xp}}} = C_{B_{int_x}}$

$C_{B_{f_{xp}}}$ ... final concentration of product B while purifying the intermediate produced from reaction x

$hot\ water_{xp}$ ... total amount of hot water needed while purifying the intermediate produced from reaction x

Equations 4.19 - 4.22 represent the dynamic mass and energy balances for the purificators, while Equation 4.23 ensures that the purification stops only after the desired concentration of the product B is reached. Equation 4.24 represents the total amount of hot water utilized during the purification. Besides, it is assumed that the minimum batch size required to start operating the purificators is 0.2 m^3. The data used for the purificators is given Table 4.2. The STN representation of this process is shown in Figure 4.4 and the corresponding basic data for the units and the states involved is presented in Table 4.3. Additionally, the following costs are assumed for the running the process:

1. The running cost of the reactor is 1.2 MU per hour.
2. The cost of coolant is 7.0 MU per m^3.
3. The running cost of the purificator is 2.0 MU per hour.
4. The cost of hot water is 20.0 MU per m^3.

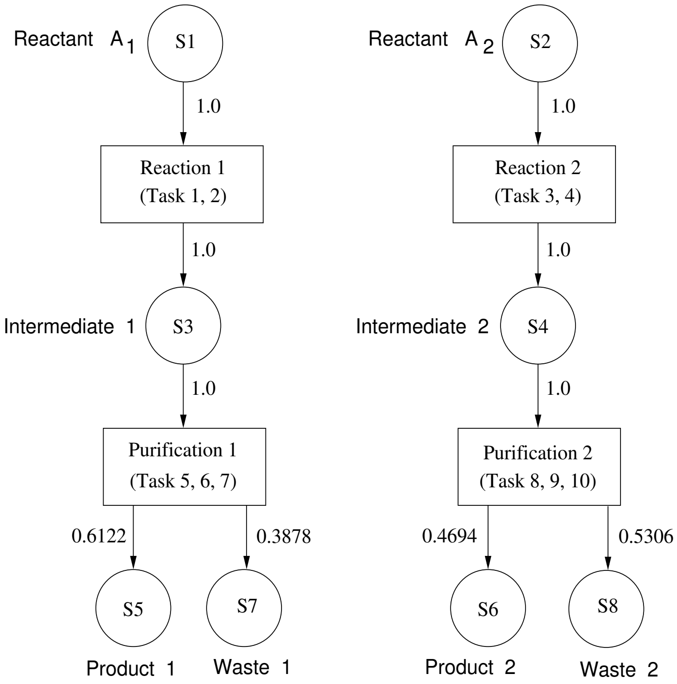

Figure 4.4: State-task-network representation of the application example.

The objective for this example is maximization of overall profit for the plant over a fixed

Table 4.2: Data used for the purificators in the application example.

V_m = 0.02 m^3	V_J = 0.302 m^3	T_{jin} = 336.0 K
A_i = 3.3 m^2	A_o = 3.3 m^2	$F_{J_{xp}}(t) \in$ [0.0, 9.0] m^3/h
$T_{m_{xp}}(t=0)$ = 336.0 K	$T_{J_{xp}}(t=0)$ = 336.0 K	$C_{B_{xp}}(t=0)$ = $C_{B_{0_{xp}}}$
$V_{xp}(t=0)$ = $V_{0_{xp}}$	H_{latent_1} = 792.0 J/kg	H_{latent_2} = 673.0 J/kg
$C_{B_{f_{1p}}}$ = 0.98 $kmol/m^3$	$C_{B_{f_{2p}}}$ = 0.98 $kmol/m^3$	

Table 4.3: Data for example 2.

Unit(j)	Capacity(m^3)	Suitability(task i)
Reactor R1(j=1)	1.2	Reactions 1(i=1) & 2(i=3)
Reactor R2(j=2)	0.6	Reactions 1(i=2) & 2(i=4)
Purificator P1(j=3)	0.6	Purifications 1(i=5) & 2(i=8)
Purificator P2(j=4)	0.6	Purifications 1(i=6) & 2(i=9)
Purificator P3(j=5)	0.6	Purifications 1(i=7) & 2(i=10)
State(s)	**initial amount(m^3)**	**price(MU per m^3)**
Reactant A_1(s=1)	10.0	50.0
Reactant A_2(s=2)	10.0	45.0
Intermediate 1(s=3)	0.0	0.0
Intermediate 2(s=4)	0.0	0.0
Product 1(s=5)	0.0	540.0
Product 2(s=6)	0.0	515.0
Waste 1(s=7)	0.0	0.0
Waste 2(s=8)	0.0	0.0

makespan of 6 hours, where the overall profit is defined as follows:

$$\begin{aligned}
Profit &= (price\ of\ products) - (price\ of\ reactants) \\
&- (running\ cost\ of\ the\ reactors) \\
&- (running\ cost\ of\ the\ purificators) \\
&- (cost\ of\ coolant\ needed\ for\ the\ reactions) \\
&- (cost\ of\ hot\ water\ needed\ for\ the\ purifications)
\end{aligned}$$

It is assumed that a minimum of 0.1 m^3 of each product should be produced within the given time horizon so as to satisfy the market requirement. Additionally, the following cleaning restrictions are assumed during the operation of the plant:

1. A cleaning time of 0.65 hour and 0.4 hour is needed on the reactors R1 and R2 respectively between every different reaction tasks that are being performed on these reactors.

2. A cleaning time of 0.4 hour is needed on the purificators between every different purification tasks that are being executed on these purificators.

4.1 Control via the improved approach

In this section, the IA is applied to the control problem of the above mentioned plant. The various steps involved in the control problem formulation for this plant are presented in the following:

Determination of suitable recipe functions

Reactors :

As described in chapter 3, the suitable recipe functions for the reactors are obtained by solving the following two SBO problems:

SBO problem 1

Here, the minimum processing durations (dur_0) for different batch sizes and for each reaction x on each reactor r are determined by solving the following optimization problem :

$$minimize \quad dur_0 \tag{4.25}$$

subject to

$$Equations \;\; \text{4.1 - 4.16}$$

The corresponding optimization results are presented in Tables 4.4 and 4.5.

Table 4.4: Minimum processing durations for different batch sizes for reaction 1 on reactors 1 and 2.

reaction1 on reaction1		reaction1 on reaction2	
vol (m^3)	dur_0 (h)	vol (m^3)	dur_0 (h)
0.4	2.3188	0.2	2.2877
0.6	2.3578	0.3	2.3103
$\vdots$	$\vdots$	$\vdots$	$\vdots$
1.2	2.4714	0.6	2.3955

The dependence of the minimum processing duration on the batch size for each reaction on each reactor, which is determined via suitable polynomial fitting of the data presented

Table 4.5: Minimum processing durations for different batch sizes for reaction 2 on reactors 1 and 2.

reaction1 on reaction1		reaction1 on reaction2	
vol (m^3)	dur_0 (h)	vol (m^3)	dur_0 (h)
0.4	3.1347	0.2	3.1312
0.6	3.1392	0.3	3.1365
$\vdots$	$\vdots$	$\vdots$	$\vdots$
1.2	3.1493	0.6	3.1482

in Tables 4.4 and 4.5, are expressed by Equations 4.26 - 4.29. The corresponding polynomial plots along with their residuals are shown in Figures 4.5 - 4.8.

$$dur_0(1,1,n) = \begin{cases} 0, & vol(1,1,n) = 0 \\ 2.239 + 0.2035 \cdot vol(1,1,n) & \\ -0.008 \cdot vol(1,1,n)^2, & vol(1,1,n) > 0 \end{cases} \tag{4.26}$$

$$dur_0(2,2,n) = \begin{cases} 0, & vol(2,2,n) = 0 \\ 2.284 - 0.1926 \cdot vol(2,2,n) & \\ +1.249 \cdot vol(2,2,n)^2 - 1.033 \cdot vol(2,2,n)^3, & vol(2,2,n) > 0 \end{cases} \tag{4.27}$$

$$dur_0(3,1,n) = \begin{cases} 0, & vol(3,1,n) = 0 \\ 3.12 + 0.03925 \cdot vol(3,1,n) & \\ -0.005 \cdot vol(3,1,n)^2 - 0.00625 \cdot vol(3,1,n)^3, & vol(3,1,n) > 0 \end{cases} \tag{4.28}$$

$$dur_0(4,2,n) = \begin{cases} 0, & vol(4,2,n) = 0 \\ 3.108 + 0.1718 \cdot vol(4,2,n) & \\ -0.335 \cdot vol(4,2,n)^2 + 0.2667 \cdot vol(4,2,n)^3, & vol(4,2,n) > 0 \end{cases} \tag{4.29}$$

SBO problem 2

The minimum amount of coolant Qr required for different batch sizes over different processing durations and for each reaction x on each reactor r is determined in this step by

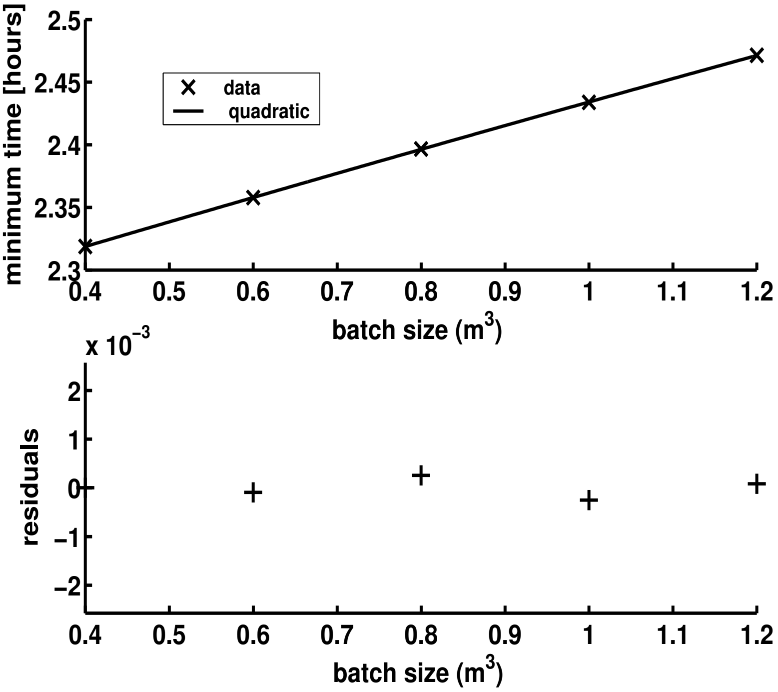

Figure 4.5: Plot of the polynomial given in Equation 4.26.

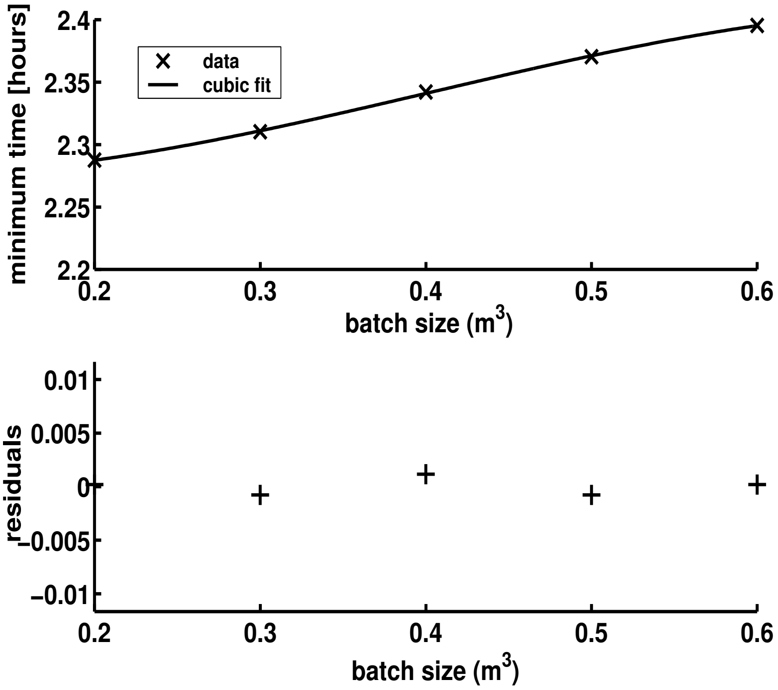

Figure 4.6: Plot of the polynomial given in Equation 4.27.

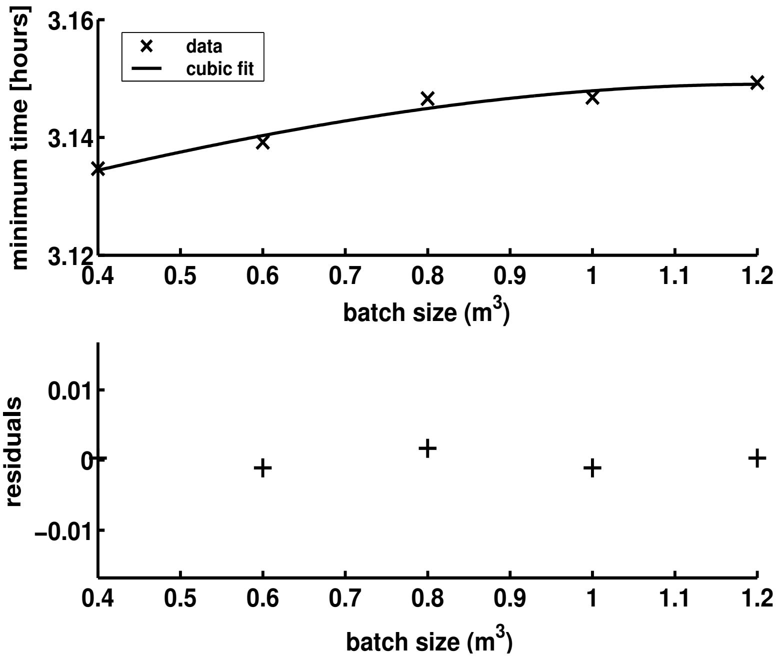

Figure 4.7: Plot of the polynomial given in Equation 4.28.

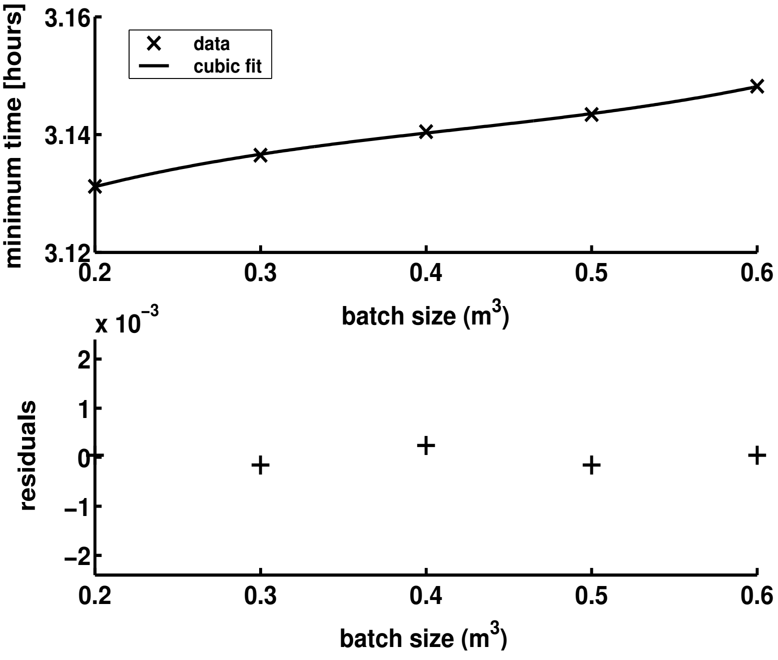

Figure 4.8: Plot of the polynomial given in Equation 4.29.

solving the following SBO problem:

$$minimize \quad coolant \tag{4.30}$$

subject to

$$Equations \;\; 4.1 - 4.16$$

The results obtained thereby are presented in Tables 4.6 - 4.9 and some of the corresponding optimal coolant profiles are shown in Figures 4.9 - 4.12.

Table 4.6: Data corresponding to optimal coolant profiles for different batch sizes and for reaction 1 on reactor 1.

0.4 m^3		0.6 m^3		…	1.2 m^3	
dur $(hours)$	Qr (m^3)	dur $(hours)$	Qr (m^3)	… …	dur $(hours)$	Qr (m^3)
2.3188	2.1708	2.3578	3.0095	…	2.4714	5.7049
2.5	1.4533	2.5	2.2706	…	2.5	5.2003
2.75	1.3297	2.75	1.9027	…	2.75	3.9715
⋮	⋮	⋮	⋮	…	⋮	⋮
6.0	0.8966	6.0	1.2720	…	6.0	2.6634

Table 4.7: Data corresponding to optimal coolant profiles for different batch sizes and for reaction 1 on reactor 2.

0.2 m^3		0.3 m^3		…	0.6 m^3	
dur $(hours)$	Qr (m^3)	dur $(hours)$	Qr (m^3)	… …	dur $(hours)$	Qr (m^3)
2.2877	1.3314	2.3103	1.7804	…	2.3955	3.4328
2.5	0.8229	2.5	1.1323	…	2.5	2.1663
2.75	0.6459	2.75	0.9396	…	2.75	1.8782
⋮	⋮	⋮	⋮	…	⋮	⋮
6.0	0.4407	6.0	0.6386	…	6.0	1.2649

Table 4.8: Data corresponding to optimal coolant profiles for different batch sizes and for reaction 2 on reactor 1.

0.4 m^3		0.6 m^3		…	1.2 m^3	
dur $(hours)$	Qr (m^3)	dur $(hours)$	Qr (m^3)	…	dur $(hours)$	Qr (m^3)
3.1347	1.7286	3.1392	2.4370	…	3.1493	5.4748
3.25	1.2381	3.25	1.7988	…	3.25	3.8139
3.5	0.9386	3.5	1.4022	…	3.5	3.1063
⋮	⋮	⋮	⋮	…	⋮	⋮
6.0	0.3379	6.0	0.6445	…	6.0	1.8348

Table 4.9: Data corresponding to optimal coolant profiles for different batch sizes and for reaction 2 on reactor 2.

0.2 m^3		0.3 m^3		…	0.6 m^3	
dur $(hours)$	Qr (m^3)	dur $(hours)$	Qr (m^3)	…	dur $(hours)$	Qr (m^3)
3.1312	0.8828	3.1365	1.2227	…	3.1405	1.6087
3.25	0.6302	3.25	0.9003	…	3.25	1.1920
3.5	0.4767	3.5	0.6975	…	3.5	0.9365
⋮	⋮	⋮	⋮	…	⋮	⋮
6.0	0.1541	6.0	0.2977	…	6.0	0.4529

The remaining recipe functions for the reactors are determined by using the data presented in Tables 4.6 - 4.9 and are expressed by Equations 4.31 - 4.42.

$$Qr(1,1,n) = \begin{cases} 0, & vol(1,1,n) = 0 \\ (9.1126 + 10.3376 \cdot vol(1,1,n) & \\ -7.0865 \cdot dur(1,1,n) + 1.3882 \cdot vol(1,1,n)^2 & \\ -3.9990 \cdot vol(1,1,n) \cdot dur(1,1,n) & \\ +1.8520 \cdot dur(1,1,n)^2 - 0.1427 \cdot vol(1,1,n)^3 & \\ -0.0431 \cdot vol(1,1,n)^2 \cdot dur(1,1,n) & \\ +0.4020 \cdot vol(1,1,n) \cdot dur(1,1,n)^2 & \\ -0.1521 \cdot dur(1,1,n)^3), & vol(1,1,n) > 0 \end{cases} \tag{4.31}$$

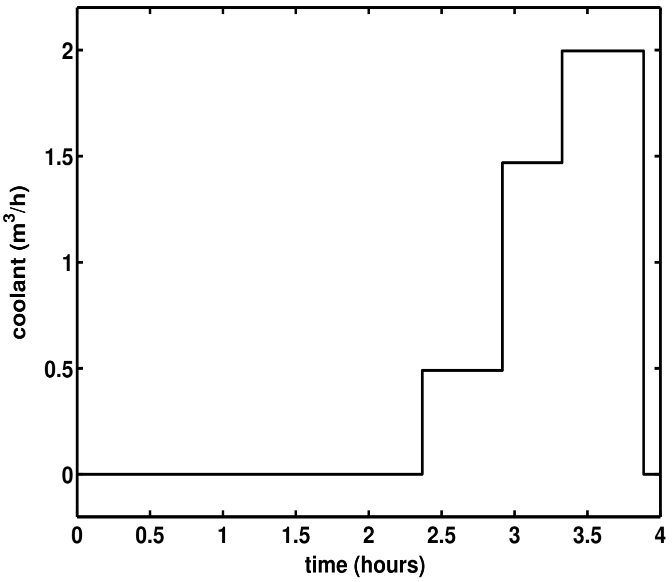

Figure 4.9: Optimal coolant profile corresponding to a batch size of 0.8 m^3 over a processing duration of 4.0 h for reaction 1 on reactor 1.

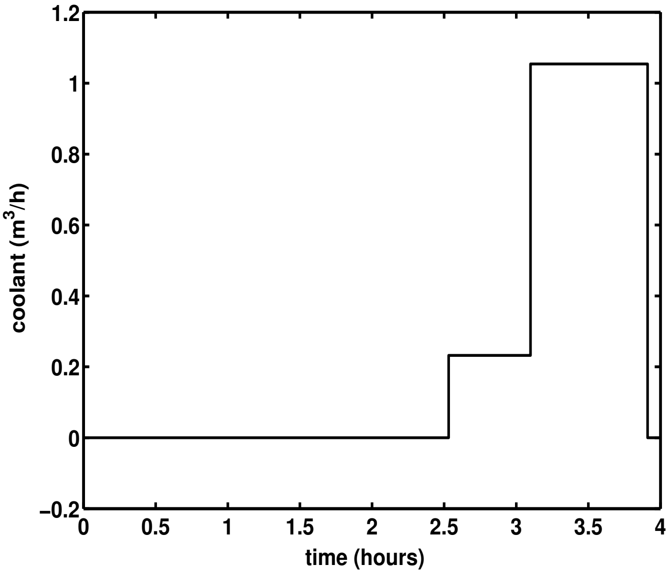

Figure 4.10: Optimal coolant profile corresponding to a batch size of 0.4 m^3 over a processing duration of 4.0 h for reaction 1 on reactor 2.

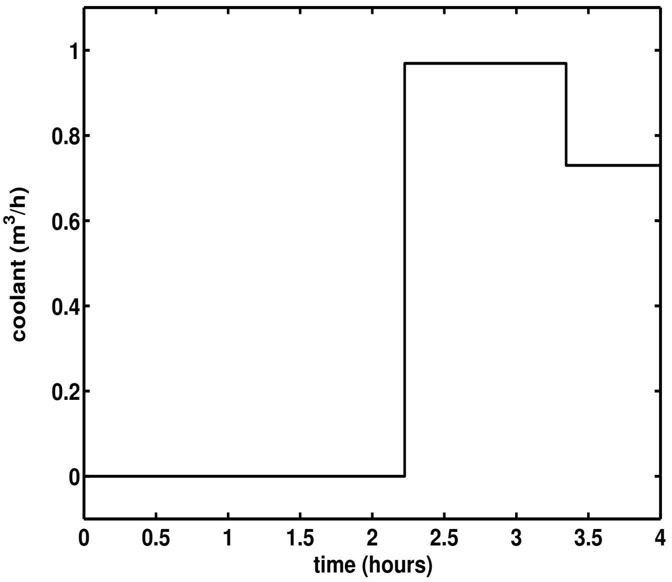

Figure 4.11: Optimal coolant profile corresponding to a batch size of 0.8 m^3 over a processing duration of 4.0 h for reaction 2 on reactor 1.

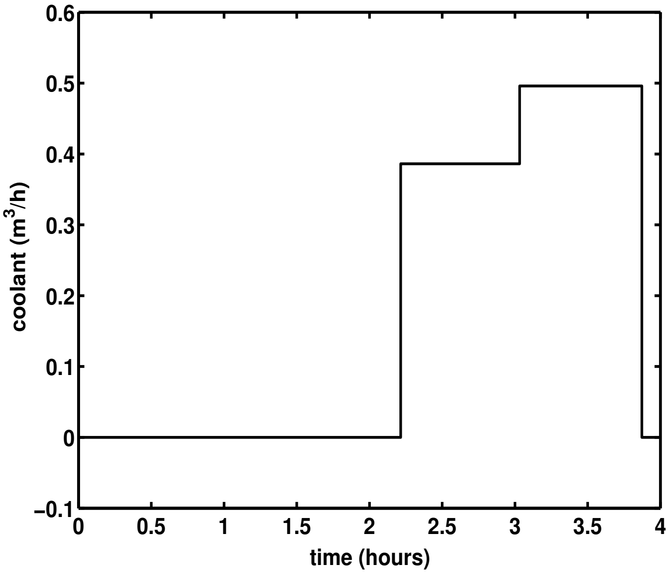

Figure 4.12: Optimal coolant profile corresponding to a batch size of 0.4 m^3 over a processing duration of 4.0 h for reaction 2 on reactor 2.

$$dur(1,1,n) = 0, \quad \forall\, vol(1,1,n) = 0 \tag{4.32}$$

$$dur(1,1,n) \geq dur_0(1,1,n) \ + \ \delta(1,1,n), \quad \forall\, vol(1,1,n) > 0 \tag{4.33}$$

$$Qr(2,2,n) = \begin{cases} 0, & vol(2,2,n) = 0 \\ (6.6247 + 16.5065 \cdot vol(2,2,n) & \\ -5.5512 \cdot dur(2,2,n) - 1.6214 \cdot vol(2,2,n)^2 & \\ -5.9626 \cdot vol(2,2,n) \cdot dur(2,2,n) & \\ +1.4732 \cdot dur(2,2,n)^2 + 1.9096 \cdot vol(2,2,n)^3 & \\ +0.1732 \cdot vol(2,2,n)^2 \cdot dur(2,2,n) & \\ +0.5838 \cdot vol(2,2,n) \cdot dur(2,2,n)^2 & \\ -0.1215 \cdot dur(2,2,n)^3), & vol(2,2,n) > 0 \end{cases} \tag{4.34}$$

$$dur(2,2,n) = 0, \quad \forall\, vol(2,2,n) = 0 \tag{4.35}$$

$$dur(2,2,n) \geq dur_0(2,2,n) \ + \ \delta(2,2,n), \quad \forall\, vol(2,2,n) > 0 \tag{4.36}$$

$$Qr(3,1,n) = \begin{cases} 0, & vol(3,1,n) = 0 \\ (26.4196 + 12.9844 \cdot vol(3,1,n) & \\ -17.8010 \cdot dur(3,1,n) + 3.3760 \cdot vol(3,1,n)^2 & \\ -5.2601 \cdot vol(3,1,n) \cdot dur(3,1,n) & \\ +3.9662 \cdot dur(3,1,n)^2 + 0.6105 \cdot vol(3,1,n)^3 & \\ -0.8878 \cdot vol(3,1,n)^2 \cdot dur(3,1,n) & \\ +0.6157 \cdot vol(3,1,n) \cdot dur(3,1,n)^2 & \\ -0.2927 \cdot dur(3,1,n)^3), & vol(3,1,n) > 0 \end{cases} \tag{4.37}$$

$$dur(3,1,n) = 0, \quad \forall\, vol(3,1,n) = 0 \tag{4.38}$$

$$dur(3,1,n) \geq dur_0(3,1,n) \ + \ \delta(3,1,n), \quad \forall\, vol(3,1,n) > 0 \tag{4.39}$$

$$Qr(4,2,n) = \begin{cases} 0, & vol(4,2,n) = 0 \\ (13.7922 + 12.7653 \cdot vol(4,2,n) & \\ -9.2228 \cdot dur(4,2,n) + 4.4099 \cdot vol(4,2,n)^2 & \\ -4.9520 \cdot vol(4,2,n) \cdot dur(4,2,n) & \\ +2.0393 \cdot dur(4,2,n)^2 - 1.3518 \cdot vol(4,2,n)^3 & \\ -0.3581 \cdot vol(4,2,n)^2 \cdot dur(4,2,n) & \\ +0.4864 \cdot vol(4,2,n) \cdot dur(4,2,n)^2 & \\ -0.1477 \cdot dur(4,2,n)^3), & vol(4,2,n) > 0 \end{cases} \tag{4.40}$$

$$dur(4,2,n) = 0, \quad \forall\, vol(4,2,n) = 0 \tag{4.41}$$

$$dur(4,2,n) \geq dur_0(4,2,n) \; + \; \delta(4,2,n), \quad \forall \, vol(4,2,n) > 0 \tag{4.42}$$

where, the values for $\delta(i,j,n)$ in the Equations 4.33, 4.36, 4.39 and 4.42 correspond to the largest residuals below zero in the Figures 4.5 - 4.8, respectively and are given as follows:

$$\delta(1,1,n) = 2.5143\text{e-}4, \quad \delta(2,2,n) = 7.7714\text{e-}4$$
$$\delta(3,1,n) = 1.12\text{e-}3, \quad \delta(4,2,n) = 1.6\text{e-}4$$

Third order polynomial regression of the data presented in Tables 4.6 - 4.9 was carried out to obtain the polynomials expressed by Equations 4.31, 4.34, 4.37 and 4.40, respectively. The respective plots of these polynomials are shown in Figures 4.13 - 4.16.

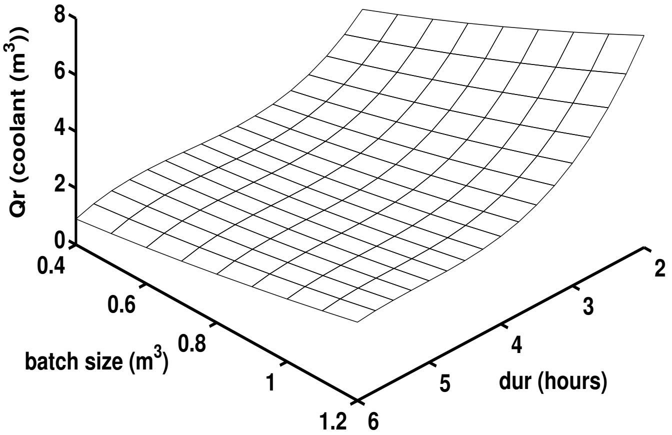

Figure 4.13: Plot of the third order polynomial given in Equation 4.31.

Purificators :

The suitable recipe functions for the purificators are obtained by solving the following two SBO problems.

SBO problem 1

This step involves determination of the minimum processing duration (dur_0) for different batch sizes and for each intermediate produced from reaction x by solving the following optimization problem.

$$minimize \quad dur_0 \tag{4.43}$$

subject to

$$Equations \;\; \text{4.19 - 4.24}$$

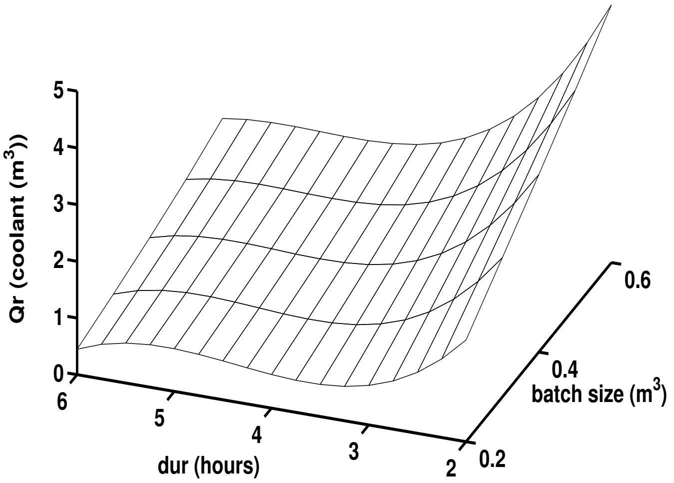

Figure 4.14: Plot of the third order polynomial given in Equation 4.34.

The corresponding optimization results are presented in Table 4.10. These results are then used to determine the dependence of the minimum processing duration on the batch size for each purification task on each purificator, which are expressed by Equations 4.44 - 4.49. Figures 4.17 and 4.18 present the corresponding polynomial plots along with their residuals.

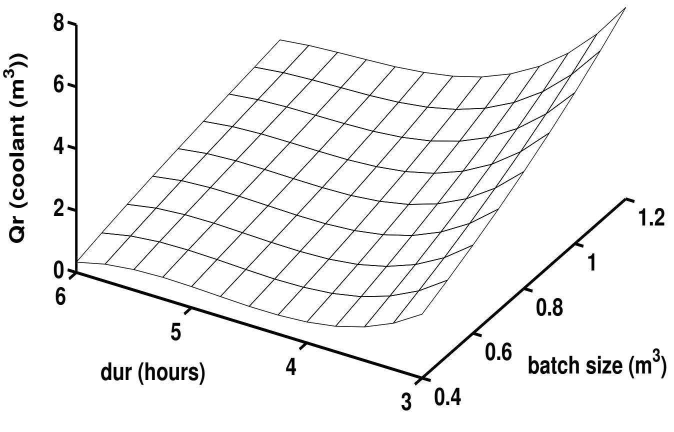

Figure 4.15: Plot of the third order polynomial given in Equation 4.37.

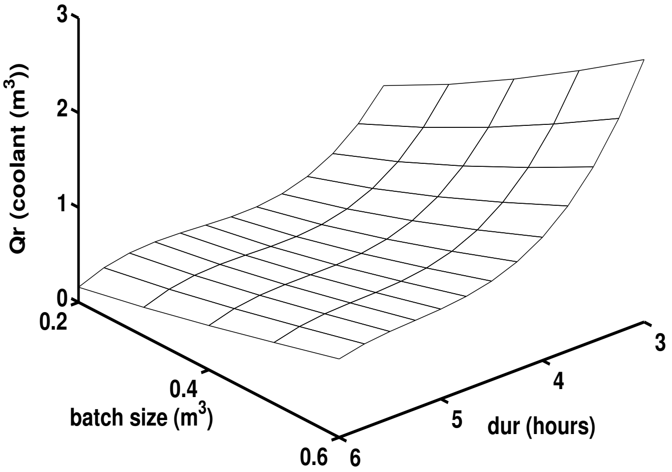

Figure 4.16: Plot of the third order polynomial given in Equation 4.40.

Table 4.10: Minimum processing durations for different batch sizes for purification 1 and 2 on each purificator.

purification 1		purification 2	
vol (m^3)	dur_0 $(hours)$	vol (m^3)	dur_0 $(hours)$
0.2	0.3922	0.2	0.7988
0.3	0.5938	0.3	1.2041
$\vdots$	$\vdots$	$\vdots$	$\vdots$
0.6	1.1994	0.6	2.4197

$$dur_0(5,3,n) = \begin{cases} 0, & vol(5,3,n) = 0 \\ -0.01102 + 2.015 \cdot vol(5,3,n) & \\ +0.003571 \cdot vol(5,3,n)^2, & vol(5,3,n) > 0 \end{cases} \tag{4.44}$$

$$dur_0(6,4,n) = \begin{cases} 0, & vol(6,4,n) = 0 \\ -0.01102 + 2.015 \cdot vol(6,4,n) & \\ +0.003571 \cdot vol(6,4,n)^2, & vol(6,4,n) > 0 \end{cases} \tag{4.45}$$

$$dur_0(7,5,n) = \begin{cases} 0, & vol(7,5,n) = 0 \\ -0.01102 + 2.015 \cdot vol(7,5,n) & \\ +0.003571 \cdot vol(7,5,n)^2, & vol(7,5,n) > 0 \end{cases} \tag{4.46}$$

$$dur_0(8,3,n) = \begin{cases} 0, & vol(8,3,n) = 0 \\ -0.01222 + 4.057 \cdot vol(8,3,n) & \\ -0.01143 \cdot vol(8,3,n)^2 & \\ +0.008333 \cdot vol(8,3,n)^3, & vol(8,3,n) > 0 \end{cases} \tag{4.47}$$

$$dur_0(9,4,n) = \begin{cases} 0, & vol(9,4,n) = 0 \\ -0.01222 + 4.057 \cdot vol(9,4,n) & \\ -0.01143 \cdot vol(9,4,n)^2 & \\ +0.008333 \cdot vol(9,4,n)^3, & vol(9,4,n) > 0 \end{cases} \tag{4.48}$$

$$dur_0(10,5,n) = \begin{cases} 0, & vol(10,5,n) = 0 \\ -0.01222 + 4.057 \cdot vol(10,5,n) & \\ -0.01143 \cdot vol(10,5,n)^2 & \\ +0.008333 \cdot vol(10,5,n)^3, & vol(10,5,n) > 0 \end{cases} \tag{4.49}$$

SBO problem 2

The minimum amount of hot water Qr required for different batch sizes over different processing durations and for each purification task on each purificator is determined in this step by solving the following SBO problem. The results obtained thereby are presented in Tables 4.11 and 4.12 and some of the optimal hot water profiles are presented in Figures 4.19 and 4.20.

$$minimize \quad hot\ water \tag{4.50}$$

subject to

$$Equations \quad \text{4.19 - 4.24}$$

The remaining recipe functions for the purificators are determined by using the data presented above and are given by Equations 4.51 - 4.68. The polynomials in these equations are obtained via third order polynomial regression of the data presented in Tables 4.11 and 4.12 and the corresponding polynomial plots are presented in Figures

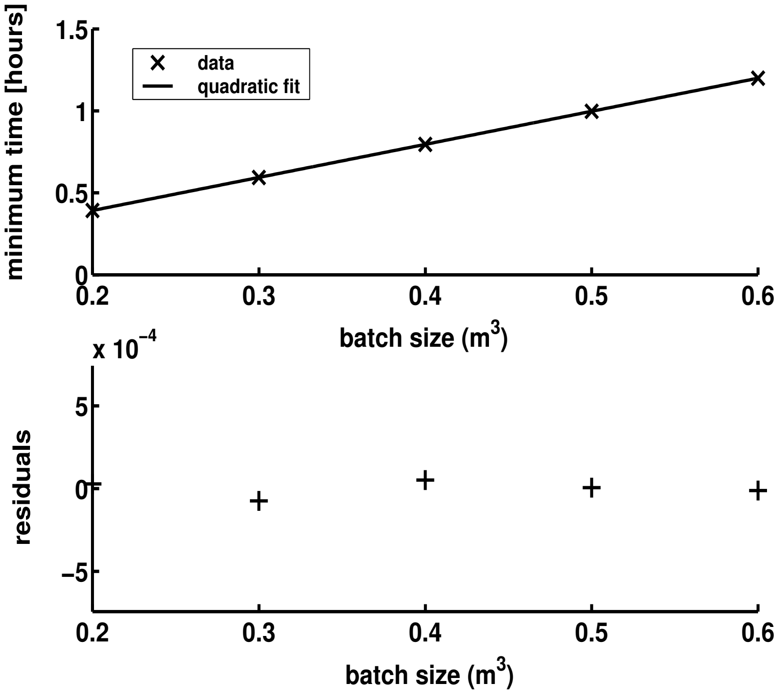

Figure 4.17: Plot of the polynomial given in Equations 4.44 - 4.46.

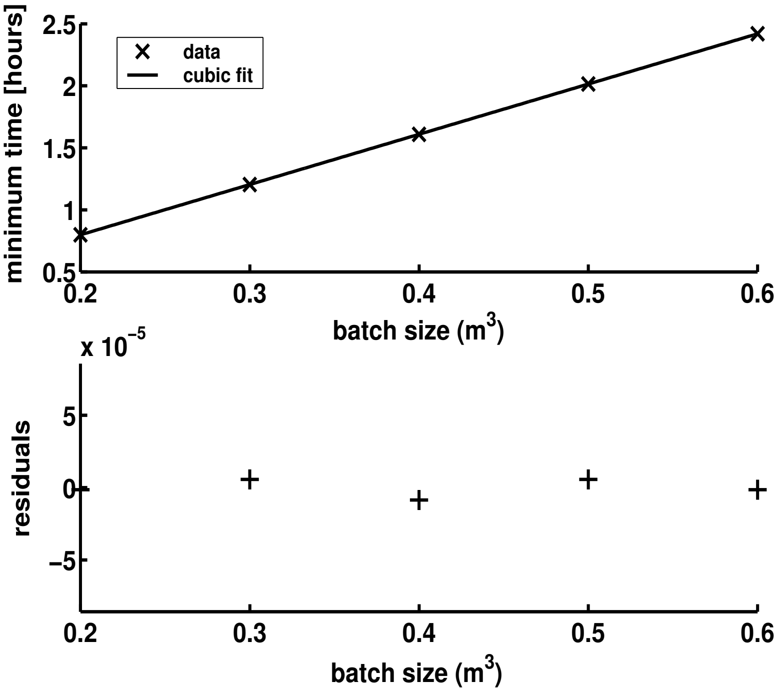

Figure 4.18: Plot of the polynomial given in Equations 4.47 - 4.49.

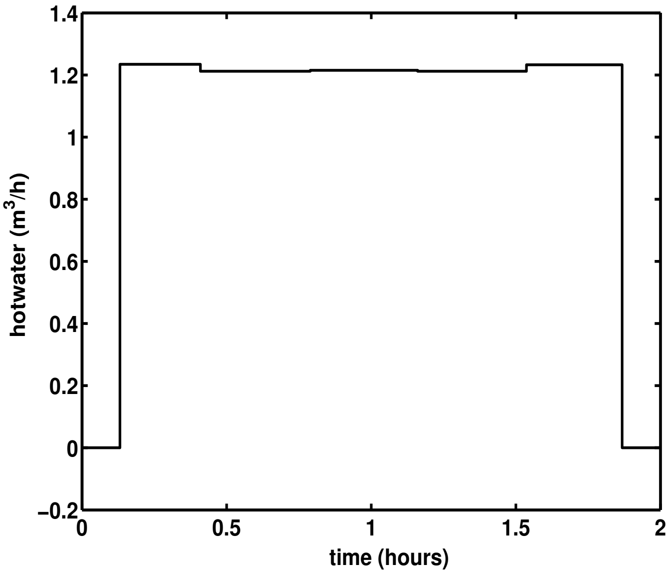

Figure 4.19: Optimal hot water profile corresponding to a batch size of 0.4 m^3 over a processing duration of 2.0 h for purification 1.

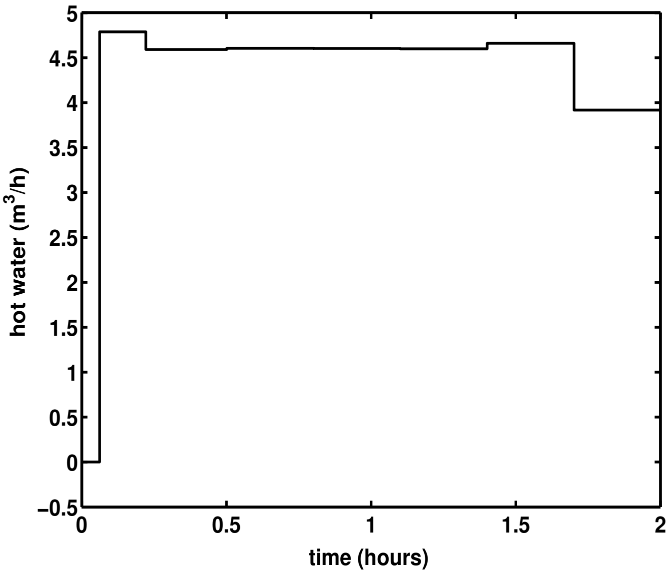

Figure 4.20: Optimal hot water profile corresponding to a batch size of 0.4 m^3 over a processing duration of 2.0 h for purification 2.

Table 4.11: Data corresponding to the optimal hot water profiles for different batch sizes and for purification 1 on each purificator.

0.2 m^3		0.3 m^3		…	0.6 m^3	
dur $(hours)$	Qr (m^3)	dur $(hours)$	Qr (m^3)	… …	dur $(hours)$	Qr (m^3)
0.3922	3.5300	0.5938	5.3439	…	1.1994	10.7946
0.5	1.6888	0.75	2.8389	…	1.25	9.2635
0.75	1.0068	1.0	1.9504	…	1.5	6.2725
⋮	⋮	⋮	⋮	…	⋮	⋮
3.0	0.6298	3.0	1.2135	…	3.0	3.4105

Table 4.12: Data corresponding to the optimal hot water profiles for different batch sizes and for purification 2 on each purificator.

0.2 m^3		0.3 m^3		…	0.6 m^3	
dur $(hours)$	Qr (m^3)	dur $(hours)$	Qr (m^3)	… …	dur $(hours)$	Qr (m^3)
0.7988	7.1891	1.2041	10.8368	…	2.4197	21.7772
1.0	4.0275	1.25	9.4022	…	2.5	19.5366
1.25	2.9817	1.5	6.3319	…	2.75	15.6944
⋮	⋮	⋮	⋮	…	3.0	13.5338
3.0	1.8903	3.0	3.5680	…		

4.21 and 4.22.

$$Qr(5,3,n) = \begin{cases} 0, & vol(5,3,n) = 0 \\ (1.3977 + 15.7615 \cdot vol(5,3,n) & \\ -4.6956 \cdot dur(5,3,n) + 77.5861 \cdot vol(5,3,n)^2 & \\ -35.0575 \cdot vol(5,3,n) \cdot dur(5,3,n) & \\ +5.2738 \cdot dur(5,3,n)^2 - 6.9635 \cdot vol(5,3,n)^3 & \\ -23.0297 \cdot vol(5,3,n)^2 \cdot dur(5,3,n) & \\ +10.4108 \cdot vol(5,3,n) \cdot dur(5,3,n)^2 & \\ -1.3069 \cdot dur(5,3,n)^3), & vol(5,3,n) > 0 \end{cases} \tag{4.51}$$

$$dur(5,3,n) = 0, \quad \forall\, vol(5,3,n) = 0 \tag{4.52}$$

$$dur(5,3,n) \geq dur_0(5,3,n) \; + \; \delta(5,3,n), \quad \forall\, vol(5,3,n) > 0 \tag{4.53}$$

$$Qr(6,4,n) = \begin{cases} 0, & vol(6,4,n) = 0 \\ (1.3977 + 15.7615 \cdot vol(6,4,n) & \\ -4.6956 \cdot dur(6,4,n) + 77.5861 \cdot vol(6,4,n)^2 & \\ -35.0575 \cdot vol(6,4,n) \cdot dur(6,4,n) & \\ +5.2738 \cdot dur(6,4,n)^2 - 6.9635 \cdot vol(6,4,n)^3 & \\ -23.0297 \cdot vol(6,4,n)^2 \cdot dur(6,4,n) & \\ +10.4108 \cdot vol(6,4,n) \cdot dur(6,4,n)^2 & \\ -1.3069 \cdot dur(6,4,n)^3), & vol(6,4,n) > 0 \end{cases} \tag{4.54}$$

$$dur(6,4,n) = 0, \quad \forall\, vol(6,4,n) = 0 \tag{4.55}$$

$$dur(6,4,n) \geq dur_0(6,4,n) \; + \; \delta(6,4,n), \quad \forall\, vol(6,4,n) > 0 \tag{4.56}$$

$$Qr(7,5,n) = \begin{cases} 0, & vol(7,5,n) = 0 \\ (1.3977 + 15.7615 \cdot vol(7,5,n) & \\ -4.6956 \cdot dur(7,5,n) + 77.5861 \cdot vol(7,5,n)^2 & \\ -35.0575 \cdot vol(7,5,n) \cdot dur(7,5,n) & \\ +5.2738 \cdot dur(7,5,n)^2 - 6.9635 \cdot vol(7,5,n)^3 & \\ -23.0297 \cdot vol(7,5,n)^2 \cdot dur(7,5,n) & \\ +10.4108 \cdot vol(7,5,n) \cdot dur(7,5,n)^2 & \\ -1.3069 \cdot dur(7,5,n)^3), & vol(7,5,n) > 0 \end{cases} \tag{4.57}$$

$$dur(7,5,n) = 0, \quad \forall\, vol(7,5,n) = 0 \tag{4.58}$$

$$dur(7,5,n) \geq dur_0(7,5,n) \; + \; \delta(7,5,n), \quad \forall\, vol(7,5,n) > 0 \tag{4.59}$$

$$Qr(8,3,n) = \begin{cases} 0, & vol(8,3,n) = 0 \\ (-0.0652 + 58.0882 \cdot vol(8,3,n) & \\ -5.6987 \cdot dur(8,3,n) + 257.4706 \cdot vol(8,3,n)^2 & \\ -92.8353 \cdot vol(8,3,n) \cdot dur(8,3,n) & \\ +7.4489 \cdot dur(8,3,n)^2 - 217.2730 \cdot vol(8,3,n)^3 & \\ -158.9868 \cdot vol(8,3,n)^2 \cdot dur(8,3,n) & \\ +34.7176 \cdot vol(8,3,n) \cdot dur(8,3,n)^2 & \\ -2.1984 \cdot dur(8,3,n)^3), & vol(8,3,n) > 0 \end{cases} \tag{4.60}$$

$$dur(8,3,n) = 0, \quad \forall\, vol(8,3,n) = 0 \tag{4.61}$$

$$dur(8,3,n) \geq dur_0(8,3,n) \ + \ \delta(8,3,n), \quad \forall \, vol(8,3,n) > 0 \tag{4.62}$$

$$Qr(9,4,n) = \begin{cases} 0, & vol(9,4,n) = 0 \\ (-0.0652 + 58.0882 \cdot vol(9,4,n) & \\ -5.6987 \cdot dur(9,4,n) + 257.4706 \cdot vol(9,4,n)^2 & \\ -92.8353 \cdot vol(9,4,n) \cdot dur(9,4,n) & \\ +7.4489 \cdot dur(9,4,n)^2 - 217.2730 \cdot vol(9,4,n)^3 & \\ -158.9868 \cdot vol(9,4,n)^2 \cdot dur(9,4,n) & \\ +34.7176 \cdot vol(9,4,n) \cdot dur(9,4,n)^2 & \\ -2.1984 \cdot dur(9,4,n)^3), & vol(9,4,n) > 0 \end{cases} \tag{4.63}$$

$$dur(9,4,n) = 0, \quad \forall \, vol(9,4,n) = 0 \tag{4.64}$$

$$dur(9,4,n) \geq dur_0(9,4,n) \ + \ \delta(9,4,n), \quad \forall \, vol(9,4,n) > 0 \tag{4.65}$$

$$Qr(10,5,n) = \begin{cases} 0, & vol(10,5,n) = 0 \\ (-0.0652 + 58.0882 \cdot vol(10,5,n) & \\ -5.6987 \cdot dur(10,5,n) & \\ +257.4706 \cdot vol(10,5,n)^2 & \\ -92.8353 \cdot vol(10,5,n) \cdot dur(10,5,n) & \\ +7.4489 \cdot dur(10,5,n)^2 & \\ -217.2730 \cdot vol(10,5,n)^3 & \\ -158.9868 \cdot vol(10,5,n)^2 \cdot dur(10,5,n) & \\ +34.7176 \cdot vol(10,5,n) \cdot dur(10,5,n)^2 & \\ -2.1984 \cdot dur(10,5,n)^3), & vol(10,5,n) > 0 \end{cases} \tag{4.66}$$

$$dur(10,5,n) = 0, \quad \forall \, vol(10,5,n) = 0 \tag{4.67}$$

$$dur(10,5,n) \geq dur_0(10,5,n) \ + \ \delta(10,5,n), \quad \forall \, vol(10,5,n) > 0 \tag{4.68}$$

Control problem formulation

The control problem is formulated using the suitable recipe functions determined above. The mathematical formulation remains exactly the same as in section 2.2.2. The objective function, which is maximization of the overall profit for the plant, is given by Equation 4.69.

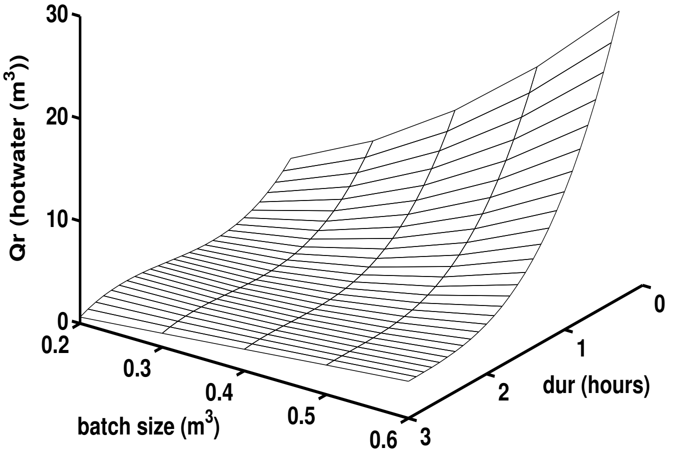

Figure 4.21: Plot of the third order polynomial given in Equations 4.51, 4.54 and 4.57.

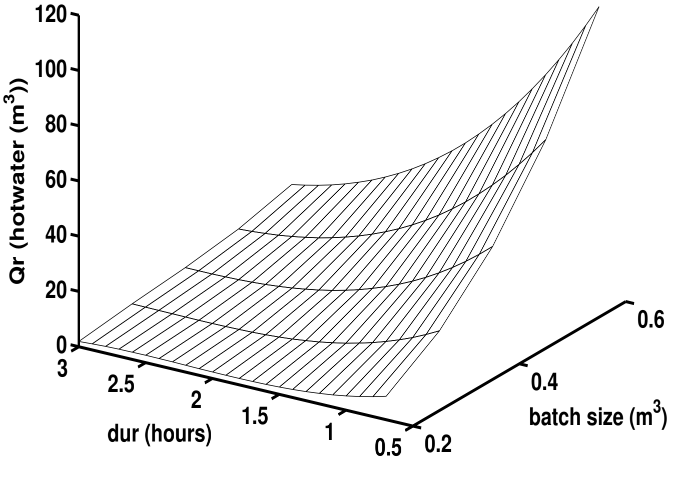

Figure 4.22: Plot of the third order polynomial given in Equations 4.60, 4.63 and 4.66.

$$
\begin{aligned}
maximize \qquad & \sum_n (540.0 \cdot d(5,n) + 515.0 \cdot d(6,n) - 50.0 \cdot (vol(1,1,n) \\
& +vol(2,2,n)) - 45.0 \cdot (vol(3,1,n) + vol(4,2,n)) - 1.2 \cdot (dur(1,1,n) \\
& +dur(3,1,n) + dur(2,2,n) + dur(4,2,n)) - 2.0 \cdot (dur(5,3,n) \\
& +dur(6,4,n) + dur(7,5,n) + dur(8,3,n) + dur(9,4,n) + dur(10,5,n)) \\
& -7.0 \cdot (Qr(1,1,n) + Qr(3,1,n) + Qr(2,2,n) + Qr(4,2,n)) \\
& -20.0 \cdot (Qr(5,3,n) + Qr(6,4,n) + Qr(7,5,n) + Qr(8,3,n) \\
& +Qr(9,4,n) + Qr(10,5,n))) \qquad (4.69)
\end{aligned}
$$

Computational result

A maximum profit of 202.851 MU is achieved over a makespan of 6 hours and the corresponding production schedule is shown in Figure 4.23. The optimal solution was found to converge at four event points and the corresponding model statistics are presented in Table 4.13.

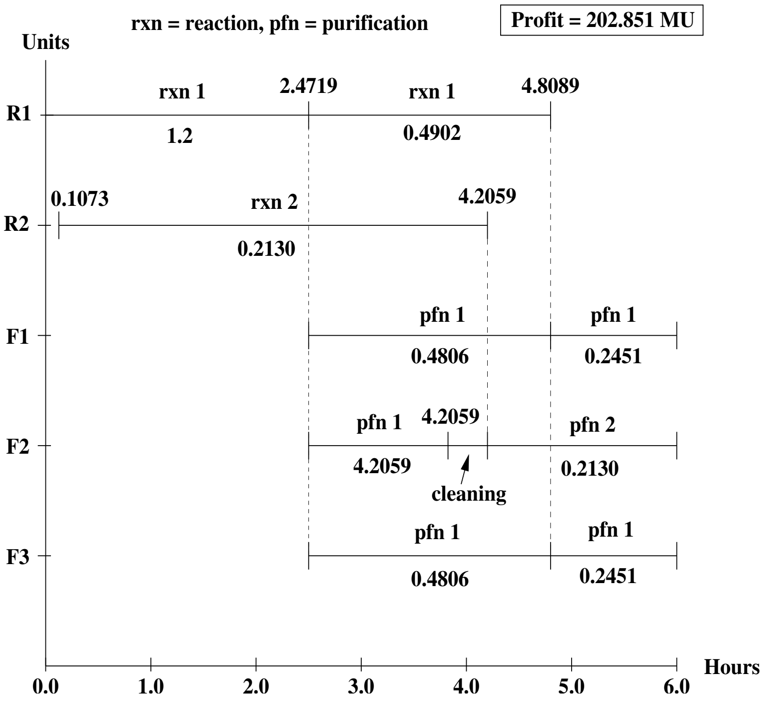

Figure 4.23: Optimal schedule obtained obtained via the IA for the application example.

Table 4.13: Model statistics corresponding to the optimal schedule for the application example.

Integer variables	40
Continuous variables	257
Equations	409
Solution (MU)	202.851
CPU time(s)	98.670

The data presented in Table 4.13 clearly highlights the effectiveness of the IA. Considering the detailed dynamics for the reaction and the purification tasks taken into account in this example, the solution time needed for the control problem is very reasonable.

4.2 Summary

In this chapter, a more realistic example with detailed process dynamics for all the tasks involved is considered. The IA for the control of MBPs, which was developed in the previous chapter, is successfully applied to this example. From the results presented in this chapter, it becomes more clear that the IA can be easily applied to the real world problems. It not only brings additional degrees of freedom into the control problem but also maintains its computational tractability.

Chapter 5

Conclusions and Perspectives

Many of the important and high value products such as fine chemicals, pharmaceuticals etc. are manufactured in MBPs. Due to the ability to respond quickly to the ever changing market demands, these plants are becoming increasingly important in the chemical manufacturing arena. The raw materials or the products associated with these plants are usually very valuable and therefore, the way these materials are handled affects the economics of the whole process very greatly. This makes the optimal control of these plants all the more important.

The optimal control problem of MBPs is a very challenging one and has been the topic of extensive research over the past few decades. The two major approaches, i.e., the SRA and the OOA for the control of MBPs are studied in this work with the help of illustrative examples. This study clearly indicates the ups and downs of both these approaches. The SRA, which leads to control problems that are relatively more computation friendly, lacks in the degrees of freedom and usually results in solutions that are far from the optimal. Besides, there are no standard guidelines available for the determination of standard production recipes, as required in the SRA. While the OOA, which should be the ideal approach for the control of MBPs, usually results in computationally intractable control problems.

The IA proposed in this work seems to be a more appropriate approach for the control of MBPs, as it offers a good mix of the number of degrees of freedom and the computational tractability of the control problem. The effectiveness of the IA is clear from the illustrative examples considered in this work. It is evident from these examples that the IA is indeed a nice trade-off between the SRA and the OOA. Further, the application example considered in this work, clearly indicates its applicability to the real world plants.

Methodologically the IA is an extension of the SRA, only differing in the way the recipes are determined. This makes the IA even more interesting as it can be used to easily upgrade all the existing SRA formulations, simply by replacing the standard production recipes with the suitable recipe functions. This property of the IA can be very instrumental, particularly for the control of very large MBPs. Control of large-scale MBPs has been studied in detail in the past and several effective SRA formulations have been proposed for this in the literature [10, 6, 23, 47]. These formulations can be easily transformed into the IA formulation, thereby improving the solutions obtained by them. Similarly, the IA can be easily adopted for upgrading the SRA formulations for the control of MBPs with intermediate due dates [21] and for the rescheduling problem of MBPs [46].

Though the IA proposed in this work seems to be a good approach for the control of MBPs, there still remains a lot to be explored further for this approach. First of all, the polynomials involved in the determination of the suitable recipe functions may not always be computation friendly. There could be cases where they might involve several local minima, which might require special handling techniques. Secondly, throughout this work, only processes involving fixed conversions and fixed inlet and outlet concentrations of the feed and product respectively have been considered. It is a known fact [8] that keeping the conversions and/or the inlet and/or outlet concentrations variable adds a large degree of flexibility to the process. Hence, the IA needs to be extended to such processes. Determination of suitable recipe functions for such processes is going to be an arduous task and may need some special techniques.

Appendix A

The State Task Network

The state task network (STN) was first introduced in the year 1993 by Kondili et. al. [24] in the context of short-term scheduling of batch operations. Prior to the introduction of the STN, the so called ”recipe networks” [39] were one of the most popular means for the graphical representation of batch processes. These recipe networks, however, involved serious ambiguities [24] when applied to complex processing structures such as the multiproduct batch plants (MBPs). In order to overcome these ambiguities of the recipe networks in a systematic fashion, the STN representation was proposed in the year 1993 and since then has been followed by several researchers [18, 28, 29] for the formulation of the control problem for the MBPs.

The STN comprises of two different types of nodes; namely, the ”state” nodes (denoted by circles) and the ”task” nodes (denoted by rectangles) connected by means of arrows. The state nodes represent the feeds, intermediates and the final products and the task nodes represent the process operations (reactions, filtrations etc.), which transform material from one or more inputs states to one or more output states. For example, in Figure A.1, task 1 transforms 50% of state S1 and 50% of state S2 into 30% of state S3 and 70% of state S4. Similarly, task 2 transforms 70% of state S4 into 35% each of states S5 and S6.

The STN unambiguously represents the flow of materials within the process. Particularly, challenging situations like the recycle streams and the production and consumption of intermediate states can be very clearly and concisely represented in these networks. Figure A.2(a) shows the state task network of a process involving a recycle stream. As per this figure, state S1 is reproduced/recovered in task 2 and recycled back. Figure A.2(b) represents a process where an intermediate state S3 is produced/recovered by task 2 and

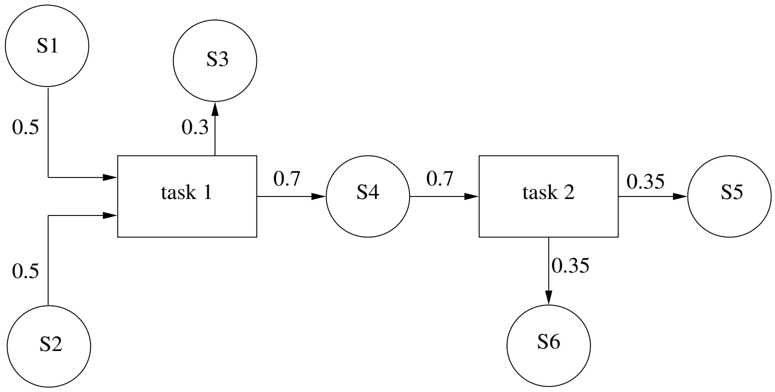

Figure A.1: An example state task network.

consumed by task 1. This situation was encountered earlier in example 2 presented in chapter 2, where the solvent represented a state similar to the state S3. This is something that could not be done so clearly with the recipe networks used earlier and is perhaps one of the strongest features of the STNs.

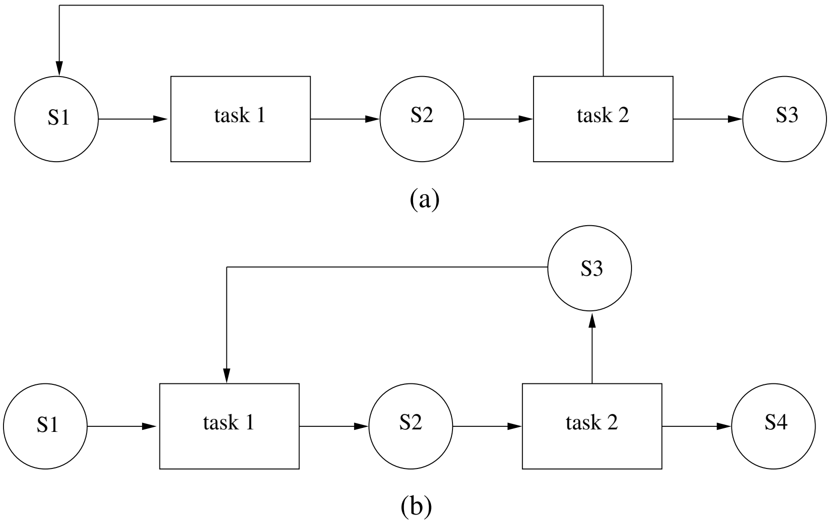

Figure A.2: State task networks representing two different processes, one with a recycle stream and the other involving an intermediate state production and consumption.

It needs to be mentioned, that the STNs need not necessarily be connected graphs. A processing structure can sometime be represented by a number of disjoint sub-graphs. This is typically the case with plants involving the production of a number of products in the same plant but not sharing any raw materials or intermediates. As an example, consider the simple plant shown in Figure A.3, where two products, B1 and B2, are produced in the same reactor from two different reactants A1 and A2. Since the two products do not share any of the reactants, the STN representation of this plant involves two disjoint sub-graphs, as shown in Figure A.4.

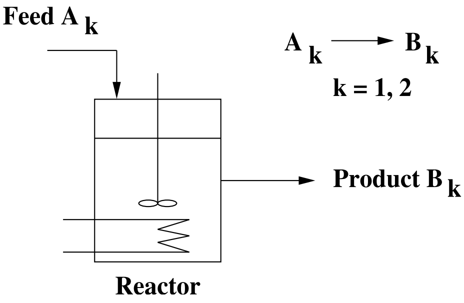

Figure A.3: An example plant.

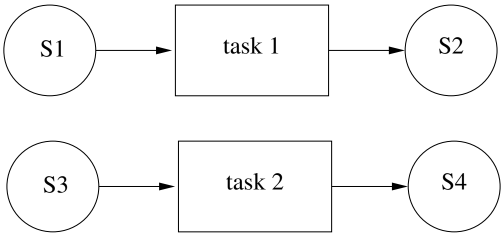

Figure A.4: State task network representation of the example plant.

The STNs are not restricted only to the batch processes but can also be used for representing the semi-continuous and continuous processes, as long as the following rules are respected:

- A task has as many input/output states as different types of input/output materials.
- Two or more streams entering or leaving the same state are necessarily of the same quality (for e.g., same temperature, composition etc.). If mixing of different streams is involved in the process, then this operation should be represented as a separate task.

In addition to the features discussed above, the STNs can be easily modified to incorporate difficult situations like the limited and unlimited interconnectivity amongst the processing units or multipurpose storage capacities. However, such situations have not been considered in this work and hence these modifications of the STNs are not discussed here. A detailed information on these modifications can be found in the original work of Kondili et. al. [24].

Appendix B

Transformation of Dynamic Optimization problem into Nonlinear Programming Problem.

This appendix presents the general transformation of the dynamic optimization (DO) problem into the nonlinear programming (NLP) problem, via the standard trapezoidal rule [17, 7].

B.1 The dynamic optimization problem

The general dynamic optimization problem for a chemical process can be written as follows:

$$\max_{z(t),\ u(t),\ dur} \gamma(z(t),\ u(t),\ z(dur)) \tag{B.1}$$

subject to

$$\frac{dz(t)}{dt} = f(z(t),\ u(t)) \tag{B.2}$$

$$h(z(t),\ u(t)) = 0 \tag{B.3}$$

$$g(z(t),\ u(t))\ \leq\ 0 \tag{B.4}$$

$$h_{ep}(z(t_{ep}),\ u(t_{ep})) = 0 \tag{B.5}$$

$$g_{ep}(z(t_{ep}),\ u(t_{ep}))\ \leq\ 0 \tag{B.6}$$

$$t\ \in\ [0,\ dur],\quad t_{ep}\ \in\ \{0,\ dur\}$$

Where, $z(t)$ and $u(t)$ represent the state and the control profile vectors respectively. Equations B.2 and B.3 represent the process model, while Equations B.4 represents path constraints. Equations B.5 and B.6 represent equality and inequality end-point constraints.

B.2 Transformation of the dynamic optimization problem into the NLP problem

The transformation of the DO into the NLP involves the following two steps:

B.2.1 Time discretization

The makespan is divided into an arbitrary number of control-intervals of unknown lengths as shown in Fig. B.1. Several time-points are defined over each control-interval as shown in Fig. B.2. The total number of time-points within each control-interval is kept same, because, consideration of a variable number of time-points depending on the length of each control-interval would call for definition of sets with variable number of elements, which in turn may numerically complicate the OC problem. The number of time-points within each control-interval should be such that the spacing between them (i.e., step(s,i) as shown in Fig. (B.2)) is sufficiently small for the accurate approximation of the differential equations. The actual necessary number of control-intervals is determined iteratively by inspecting the solutions obtained with the increasing number of control intervals.

B.2.2 The NLP formulation

As mentioned earlier, the NLP problem is formulated by using the standard trapezoidal rule. The formulation is based on the following notations:

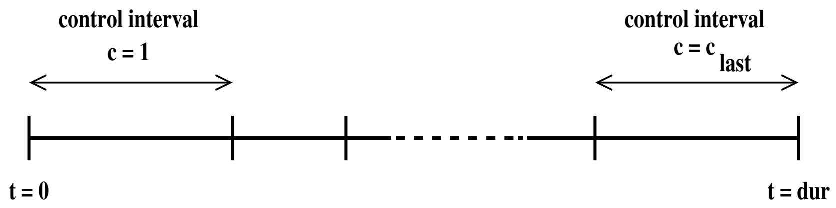

Figure B.1: Consideration of control-intervals within the makespan.

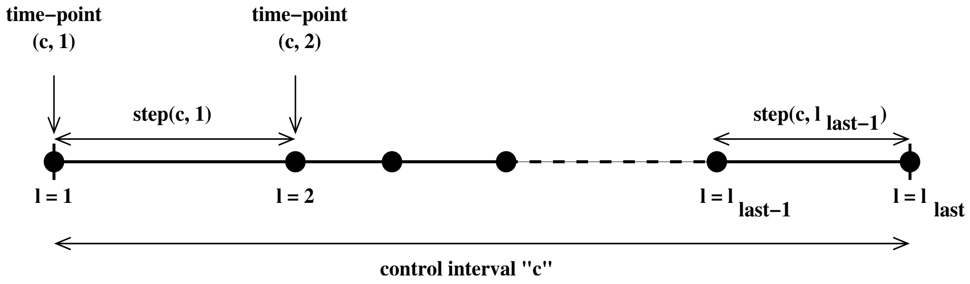

Figure B.2: Consideration of time-points within each control-interval.

Indices

index l relates to time-points

index c relates to control-intervals

Sets

L . . . set of time-points

C . . . set of control-intervals

Variables

$z(c, l)$ = value of state variables z at time-point l within control-interval c

$u(c)$ = value of control variables u within control-interval c

$step(c, l)$ = spacing between time-points l and $l + 1$ within control-interval c

The corresponding NLP problem is given as follows:

$$\max_{z(l),\, u(l),\, dur} \gamma(z(l),\ u(l),\ z(dur)) \tag{B.7}$$

subject to

$$z(c, l) = z(c, l-1) + \frac{step(c, l-1)}{2} \cdot \big(f(z(c, l-1), u(c)) + f(z(c, l), u(c))\big), \quad \forall c \in C,\ l \in L, l \geq 2 \tag{B.8}$$

$$h(z(c,l),u(c)) = 0, \quad \forall c \, \in \, C, \, l \, \in \, L \tag{B.9}$$

Equations B.8 and B.9 represent the discrete approximation of the process model given by Equations B.2 and B.3. As shown in Equation B.8, the state trajectories are approximated using piecewise-linear profiles. Whereas, piecewise-constant profiles are used for approximating the control trajectories, as these control variables mainly represent flow rates, which can sometimes be discrete as well.

$$z(c,1) = z(c-1, l_{last}), \quad \forall c \, \in \, C, \, c \, \geq \, 2 \tag{B.10}$$

It is understood from Figures B.1 and B.2 that the last time-point (i.e, l = l_{last}) of any control-interval $c - 1$ is same as the first time-point (i.e, l = 1) of the succeeding control-interval c. Hence, the continuity of the state variables over the control-intervals must be ensured. This is simply done by Equation B.10.

The path constraints can be directly imposed at every time-point within each control-interval, as expressed by Equation B.11.

$$g(z(c,l),u(c)) \leq 0, \quad \forall c \, \in \, C, \, l \, \in \, L \tag{B.11}$$

The end equality and inequality end point constraints are given by Equations B.12 - B.15.

$$h_{ep}(z(c,1),u(c)) = 0, \; c \, = \, 1 \tag{B.12}$$

$$h_{ep}(z(c,l_{last}),u(c)) = 0, \; c \, = \, c_{last} \tag{B.13}$$

$$g_{ep}(z(c,1),u(c)) \leq 0, \; c \, = \, 1 \tag{B.14}$$

$$g_{ep}(z(c,l_{last}),u(c)) \leq 0, \; c \, = \, c_{last} \tag{B.15}$$

Where, Equations B.12 and B.14 represents the initial conditions at time $t \, = \, 0$, while Equations B.15 represents the final conditions at time $t = dur$.

$$step(c,l) \leq maximum \; tolerable \; step - size, \quad \forall c \, \in \, C, \, l \, \in \, L \tag{B.16}$$

Equation B.16 ensures proper distribution of the time-points within each control-interval, so as to avoid undesirable numerical artifacts. This constraint simply implies that the maximum spacing between any two time-points is always less than or equal to the maximum tolerable step-size, which is actually needed for the accurate numerical integration of the system under consideration. Finally, the makespan is represented by Equation B.17.

$$dur = \sum_{c=1}^{c_{last}} \sum_{l=1}^{l_{last}-1} step(c,l) \tag{B.17}$$

It needs to be mentioned that equidistant time points, as used in some of the examples considered in this work, can be realized simply by using Equation B.18.

$$step(c,l) = step(c,l-1), \quad \forall c \in C,\ l \in L,\ l \leq l_{last} - 1 \tag{B.18}$$

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