PROCESS INTEGRATION AS AN OPTIMISATION TOOL IN MULTIPURPOSE BATCH PLANTS

by

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Synopsis

Heat integration to optimise energy usage becomes a possibility if a process includes both heat generating and heat consuming operations. Heat integration in batch plants has in the past been largely disregarded as utility requirements are considered less significant due to the smaller scale of batch operations compared to continuous plants. However, utility requirements in some batch plants, such as in the food and drink industries, dairies, meat processing facilities, biochemical plants and agrochemical facilities, contribute largely to their overall costs. This thesis is a continuation of the work published by Stamp and Majozi (2011) and two different aspects of heat integration in multipurpose batch plants are considered.

Firstly, wastewater minimisation constraints from the model of Adekola and Majozi (2011) were superimposed into the heat integration model of Stamp and Majozi (2011) and the simultaneous optimisation of scheduling, energy and water was considered. This has not been covered extensively in published literature as the optimisation of all three aspects of a multipurpose batch plant complicates the optimisation. The proposed simultaneous method was compared to a published sequential method and gave an improved profit of 6.78% for a multipurpose example.

Secondly, a model for the simultaneous optimisation of the schedule and energy usage in heat integrated multipurpose batch plants operated over long time horizons is presented. The method uses a cyclic scheduling solution procedure. Indirect heat integration via heat storage was included, rather than just direct heat integration. This has not been considered in long-term heat integration models in current literature. Both the heat storage size and initial heat storage temperature were also optimised. The solution obtained over 24 h using the proposed cyclic scheduling model with heat storage for a simple sequential process was compared to the result obtained from the direct solution and an error of less than 1% was achieved.

Declaration

I, Jane Dorothy Stamp, student number 04319745, declare that:

1. I understand what plagiarism is and am aware of the University's policy in this regard.
2. I declare that this thesis is my own original work. Where other people's work has been used (either from a printed source, internet or any other source), this has been properly acknowledged and referenced in accordance with departmental requirements.
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5. The work presented in this thesis has not been submitted anywhere else in partial or full fulfillment of another degree.

Student________________

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Nomenclature

Sets

C	$\{c \mid c$ = contaminant$\}$
J	$\{j \mid j$ = processing unit$\}$
J_c	$\{j_c \mid j_c$ = processing unit which may conduct tasks requiring heating$\} \subseteq J$
J_h	$\{j_h \mid j_h$ = processing unit which may conduct tasks requiring cooling$\} \subseteq J$
J_s	$\{j_s \mid j_s$ = a unit producing state $s\} \subseteq J$
J_w	$\{j_w \mid j_w$ = processing unit which requires washing after conducting a task$\} \subseteq J$
P	$\{p \mid p$ = time point$\}$
S	$\{s \mid s$ = any state$\}$
S_{in}	$\{s_{in} \mid s_{in}$ = input state into any unit$\}$
$S_{in,j}$	$\{s_{in,j} \mid s_{in,j}$ = input state to a processing unit$\} \subseteq S$
$S_{in,j}^{*}$	$\{s_{in,j}^{*} \mid s_{in,j}^{*}$ = effective state into a processing unit$\} \subseteq S_{in,j}$
$S_{in,j}^{sc}$	$\{s_{in,j}^{sc} \mid s_{in,j}^{sc}$ = task consuming state $s\} \subseteq S_{in,j}$
$S_{in,j}^{sp}$	$\{s_{in,j}^{sp} \mid s_{in,j}^{sp}$ = task which produces state s, other than a product$\} \subseteq S_{in,j}$
$S_{in,j}^{s^p}$	$\{s_{in,j}^{s^p} \mid s_{in,j}^{s^p}$ = task which produces state s, which is a product$\} \subseteq S_{in,j}$
$S_{in,j}^{usc}$	$\{s_{in,j}^{usc} \mid s_{in,j}^{usc}$ = task consuming unstable state $s\} \subseteq S_{in,j}$
$S_{in,j}^{usp}$	$\{s_{in,j}^{usp} \mid s_{in,j}^{usp}$ = task which produces unstable state $s\} \subseteq S_{in,j}$
S_{out}	$\{s_{out} \mid s_{out}$ = output state from any unit$\}$
$S_{out,j}$	$\{s_{out,j} \mid s_{out,j}$ = output state from a processing unit$\} \subseteq S$
$S_{out,j,j'}$	$\{s_{out,j,j'} \mid s_{out,j,j'}$ = recycled state from unit j to unit $j'\} \subseteq S$
S^{p}	$\{s^{p} \mid s^{p}$ = a state which is a final product$\}$

U $\{u \mid u$ = heat storage unit$\}$

Continuous variables

$B(s_{in,j}, p)$	batch size, either fixed or variable
$c_{in}(s_{in,j}, c, p)$	inlet concentration of contaminant c, to unit $j \in J_w$ at time point p
$c_{out}(s_{out,j}, c, p)$	outlet concentration of contaminant c, from unit $j \in J_w$ at time point p
$CL(s_{in,j_h}, p)$	cooling load for hot state
$\dot{CL}(s_{in,j_h}, p)$	cooling load per time, for hot state
$cs_{in}(c, p)$	inlet concentration of contaminant c, to storage at time point p
$cs_{out}(c, p)$	outlet concentration of contaminant c, from storage at time point p
$cw(s_{in,j_h}, p)$	external cooling required by unit j_h conducting the task corresponding to state s_{in,j_h} at time point p
$d(s, p)$	amount of state delivered to customers at time point p
$dur(s_{in,j}, p)$	duration of task, dependent on batch size
$extra\_cw(u)$	additional cooling required in heat storage vessel
$extra\_st(u)$	additional heating required in heat storage vessel
G_{cw}	Glover Transformation variable
G_{st}	Glover Transformation variable
H	time horizon of interest, optimisation variable for makespan minimisation problem / single cycle length for cyclic scheduling problem
$HL(s_{in,j_c}, p)$	heating load for cold state
$\dot{HL}(s_{in,j_c}, p)$	heating load per time, for cold state

K_{cw}	Reformulation-Linearisation variable
K_{st}	Reformulation-Linearisation variable
$M_B(s_{in,j}, c, p)$	mass load of contaminant c in unit $j \in J_w$ at time point p after processing $s_{in,j}$ that is added to the water stream
$m_u(s_{in,j}, p)$	amount of material processed in a unit at time point p
$m_p(s_{out,j}, p)$	amount of material produced from a unit at time point p
$mw_{in}(s_{in,j}, p)$	mass of water into unit $j \in J_w$ for washing at time point p
$mw_{out}(s_{out,j}, p)$	mass of water exiting unit $j \in J_w$ at time point p after washing
$mw_f(s_{in,j}, p)$	mass of freshwater into unit $j \in J_w$ at time point p
$mw_e(s_{out,j}, p)$	mass of effluent water from unit $j \in J_w$ at time point p
$mw_r(s_{out,j,j'}, p)$	mass of water recycled/ reused from j to unit j' $(j, j' \in J_w)$ at time point p
$ms_{in}(j, p)$	mass of water transferred from unit $j \in J_w$ to storage at time point p
$ms_{out}(j, p)$	mass of water transferred from storage to unit $j \in J_w$ at time point p
$Q(s_{in,j}, u, p)$	heat exchanged with heat storage unit u at time point p
$q(s_{in,j_h}, s_{in,j_c}, p)$	amount of heat exchanged during direct heat integration
$q_s(s, p)$	amount of state s stored at time point p
$Q_s^0(s)$	initial amount of intermediate state s stored (cyclic scheduling)
$qw_s(p)$	amount of water stored in storage at time point p
$st(s_{in,j_c}, p)$	external heating required by unit j_c conducting the task corresponding to state s_{in,j_c} at time point p
$T_0(u, p)$	initial temperature in heat storage unit u at time point p
$T_f(u, p)$	final temperature in heat storage unit u at time point p

ΔT_{cw}	temperature change required in heat storage vessel to return to the starting temperature, when additional cooling is required
ΔT_{st}	temperature change required in heat storage vessel to return to the starting temperature, when additional heating is required
T_{start}	initial temperature of heat storage at the beginning of a cycle
T_{end}	temperature of heat storage at the end of a cycle
$t_0(s_{in,j}, u, p)$	time at which heat storage unit u commences activity
$t_f(s_{in,j}, u, p)$	time at which heat storage unit u ends activity
$t_u(s_{in,j}, p)$	time at which a task starts or state is used in unit j
$t_p(s_{in,j}, p)$	time at which a task ends in unit j
$t_{out}(s_{out,j}, p)$	time at which a state is produced from unit j at time point p
$tw_{in}(s_{in,j}, p)$	time at which water enters unit $j \in J_w$ at time point p
$tw_{out}(s_{out,j}, p)$	time at which water exits unit $j \in J_w$ at time point p
$tw_r(s_{out,j,j'}, p)$	time at which water is recycled from unit j to unit j' $(j, j' \in J_w)$ at time point p
$ts_{in}(j, p)$	time at which water is transferred from unit $j \in J_w$ to storage at time point p
$ts_{out}(j, p)$	time at which water is transferred from storage to unit $j \in J_w$ at time point p
$uu(s_{in,j}, p)$	amount of material stored in unit j at time point p
$W(u)$	capacity of heat storage unit u
$\Gamma(s_{in,j}, u, p)$	Glover Transformation variable
$\Psi(s_{in,j}, u, p)$	Reformulation-Linearisation variable

Binary variables

$tt(j,p)$	binary variable associated with usage of state produced by unit j at time point p
$tt(j,s,p)$	binary variable associated with usage of state s produced by unit j at time point p if the unit produces more than one intermediate at time point p
$x(s_{in,j_c}, s_{in,j_h}, p)$	binary variable associated with heat integration between unit j_c conducting the task corresponding to state s_{in,j_c} and unit j_h conducting the task corresponding to state s_{in,j_h}, at time point p
x_{cw}	binary variable signifying that extra cooling is required in the heat storage vessel
x_{st}	binary variable signifying that extra heating is required in the heat storage vessel
$xx(s,p)$	binary variable associated with availability of storage for state s at time point p
$y(s_{in,j}, p)$	binary variable associated with usage of state s in unit j at time point p
$yw(s_{in,j}, p)$	binary variable showing usage of water in unit $j \in J_w$ at time point p
$yw_r(s_{out,j,j'}, p)$	binary variable showing reuse/ recycle of water from unit j to unit j' $(j, j' \in J_w)$ at time point p
$ys_{in}(j,p)$	binary variable showing transfer of water from unit $j \in J_w$ to storage at time point p
$ys_{out}(j,p)$	binary variable showing transfer of water from storage to unit $j \in J_w$ at time point p

$z(s_{in,j}, u, p)$	binary variable associated with heat integration between unit j conducting the task corresponding to state $s_{in,j}$ with heat storage unit u at time point p

Parameters

$A(c)$	contaminant loading
α	constant coefficient of processing time
β	variable coefficient of processing time
$CL(s_{in,j_h})$	fixed cooling load for hot state
cp_{fluid}	specific heat capacity of heat storage fluid
$cp_{state}(s_{in,j})$	specific heat capacity of state
$C_{in}^{U}(s_{in,j}, c)$	maximum inlet concentration of contaminant c in unit $j \in J_w$
$C_{out}^{U}(s_{out,j}, c)$	maximum outlet concentration of contaminant c from unit $j \in J_w$
CE	cost of effluent water treatment
CF	cost of freshwater
$Cost\_cw$	cost of cooling water
$Cost\_st$	cost of steam
$CP(s)$	selling price of product s, s = product
$CS_{out}^{o}(c)$	initial concentration of contaminant in storage
H	time horizon of interest, a parameter for profit maximisation problem
$HL(s_{in,j_c})$	fixed heating load for cold state
H^{U}	upper bound for cycle length
$M(s_{in,j}, c)$	mass load of contaminant c in unit $j \in J_w$ after processing $s_{in,j}$ that is added to the water stream

MM	any large number
$Mw^{U}(s_{in,j})$	maximum inlet water mass of unit $j \in J_w$
$\rho^{sc}_{s_{in,j}}$	portion of state s consumed by a task
$\rho^{sp}_{s_{in,j}}$	portion of state s produced by a task
$Q^{\max}(s_{in,j})$	maximum possible heating load or cooling load for a cold state or hot state, respectively
$Q^{0}_{s}(s)$	initial amount of state s stored
Q^{U}_{s}	maximum capacity of storage to store state s
Qw^{o}_{s}	initial amount of water in storage
Qw^{U}_{s}	maximum capacity of storage for water
$T(s_{in,j})$	operating temperature for processing unit j conducting the task corresponding to state $s_{in,j}$, for constant temperature processes
$T_{in}(s_{in,j})$	inlet temperature for state $s_{in,j}$
$T_{out}(s_{in,j})$	outlet temperature for state $s_{in,j}$
T^{L}	lower bound for heat storage temperature
T^{U}	upper bound for heat storage temperature
ΔT^{L}	lower bound for temperature difference in heat storage vessel
ΔT^{U}	upper bound for temperature difference in heat storage vessel
$\Delta T^{\min}$	minimum allowable thermal driving force
$\tau(s_{in,j})$	duration of the task corresponding to state $s_{in,j}$ conducted in unit j
$\tau w(s_{out,j})$	duration of washing for unit $j \in J_w$
$V^{L}_{s_{in,j}}$	minimum capacity of unit j to process a particular task
$V^{U}_{s_{in,j}}$	maximum capacity of unit j to process a particular task

V_j^U	maximum capacity of unit j
W^L	lower bound for heat storage capacity
W^U	upper bound for heat storage capacity

CHAPTER 1

INTRODUCTION

1.1 Background

In a batch process, discrete tasks follow a specific sequence or recipe, whereby raw materials are transformed to final products. The recipe includes the amounts of materials to be processed as well as the processing times of the various tasks (Majozi, 2010: 1). Batch processes are commonly used for the manufacture of products required in small quantities or for specialty and complex products of high value. Approximately half of all production facilities make use of batch processes (Stoltze *et al.*, 1995). Batch plants are also popular due to their flexible and adaptable nature, which is particularly important in volatile markets.

A batch process may either be multiproduct or multipurpose depending on how materials flow through the processing equipment (Sparrow *et al.*, 1975). In a multiproduct facility, each batch of product follows the same equipment path. In a multipurpose plant, the batches can use different pieces of equipment and need not follow a single path. Multipurpose plants are more flexible than multiproduct plants, but also more complex. Multiproduct plants are also a subset of multipurpose plants and a mathematical model used to solve a multipurpose batch problem can also be used to solve the multiproduct case. The converse, however, is not true.

Heating and cooling are necessary in most processing facilities. If a process includes operations where heat is generated and others where heat is required, heat integration becomes a possibility. Also, due to the inherent sharing of equipment by different tasks in a batch operation, process equipment needs to be cleaned and this is usually associated with large amounts of water. Depending on the washing requirements of the process units, water may be recycled or reused, leading to more efficient use of water for process equipment cleaning. This results in a reduction of both freshwater consumed as well as wastewater generated. Batch operations are generally run on a smaller scale compared to continuous operations and utility and water requirements have in the past been considered less significant. Heat integration and wastewater minimisation in batch plants have, therefore, largely been ignored. However, utility and water requirements in some batch plants, such as in the food industry, breweries, dairies, meat processing facilities, biochemical plants and agrochemical facilities, contribute largely to their overall costs. Minimising energy usage and water consumption is also influenced by the need to comply with stricter environmental regulations, reduce the effects of higher energy prices and conserve scarce environmental resources.

The application of heat integration in batch plants has been in published literature for more than two decades. The objective of heat integration is to optimise the use of energy. Heat integration may be achieved in two ways in a batch process. If the operating schedule allows an overlap in time of hot and cold units, direct heat integration may be used with both units required to be active. However, due to the time dependent nature of batch processes it may be necessary to store heat from a hot unit using an intermediate heat storage fluid and reuse this heat at a later time when it is required, resulting in indirect heat integration.

Methods for wastewater minimisation in batch plants have also been developed, although somewhat more recently. Wastewater minimisation is achieved by employing opportunities for water reuse. Water from a unit can be recycled into the same unit, reused by other units or sent to a water storage vessel. Direct water reuse refers to the use of an outlet wastewater stream from one unit into another unit, while indirect water reuse refers to the use of previously stored wastewater into a unit. A wastewater regenerator can also be used to purify wastewater to a quality where it can be reused in other operations, further increasing water reuse opportunities. Optimal scheduling and equipment use, decreased energy requirements and wastewater reduction can have a significant effect on the efficiency and revenue of a batch plant.

This thesis is a continuation of the work published by Stamp and Majozi (2011). The flexibility of the previous model is highlighted by considering two different aspects with a focus on heat integration. Firstly, wastewater minimisation constraints from the model of Adekola and Majozi (2011) were superimposed into the scheduling and heat integration model and as such the simultaneous optimisation of scheduling, energy and water was considered. This has not been covered extensively in published literature as the optimisation of all three aspects of a multipurpose batch plant complicates the optimisation. The current method was also compared to a published sequential method (Halim & Srinivasan, 2011) and this work has recently been published (Adekola *et al*., 2013). An additional paper on this topic, considering only direct heat integration and direct water reuse has also since been published (Seid & Majozi, 2014).

Secondly, a long-term heat integration technique is presented which aims to optimise energy usage in multipurpose batch plants over long time horizons. Most heat integration methods are limited to the short-term case and solution of problems over long time horizons may prove challenging or impossible with these methods. Rather than just considering direct heat integration, the proposed method also includes the concept of indirect heat integration via heat storage. This has not been considered in long-term heat integration models in current literature. As in the previous model of Stamp and Majozi (2011) for short-term heat integration, the proposed model includes the optimisation of both the initial heat storage temperature as well as the heat storage capacity. Apart from the necessary cyclic scheduling constraints, the scheduling model of Seid and Majozi (2012) has been combined with the heat integration model of Stamp and Majozi (2011). This scheduling model has shown to result in improvements in computational time as well as objective function in short-term scheduling problems.

1.2 Problem statement and objectives

Two different problems are addressed in this work. In Chapter 3, multipurpose batch plants with significant utility and water requirements are considered. Opportunities for heat integration and wastewater minimisation are explored simultaneously within the scheduling framework in order to maximise the overall profit or minimise the makespan, while minimising the external utility and water requirements. For this, the scheduling data, heat integration data and wastewater minimisation data are required. In Chapter 4, multipurpose batch plants with opportunities for heat integration which are operated over a long time horizon are considered. The objective is then to determine the optimal production schedule which maximises profit, defined as the difference between revenue and the costs of hot and cold utilities. For this, the scheduling data and heat integration data are required.

1.3 Scope

The work in this thesis considers the simultaneous optimisation of scheduling, energy and water in multipurpose batch plants. Both heat storage and wastewater storage are included, which has not been covered in literature. In addition, a cyclic scheduling model which includes both direct and indirect heat integration is developed to minimise energy in multipurpose batch plants over long time horizons. A comparison is also made to the direct solution of the long-term heat integration problem. In both models in this thesis, the heat storage capacity and initial heat storage temperature were optimised. Heat losses from the heat storage vessel were not considered in this work. The inclusion of a wastewater regenerator for the minimisation of wastewater was also not considered. Both models were applied to various problems found in literature.

1.4 Structure

The rest of this thesis contains the literature review in Chapter 2, concerning short-term scheduling, long-term scheduling and heat integration. A brief discussion on wastewater minimisation in batch plants is also included in order to highlight its importance. Chapter 3 considers the simultaneous optimisation of energy and water using a flexible scheduling framework. In Chapter 4, a technique is presented for the long-term heat integration of multipurpose batch plants using both direct heat integration as well as indirect heat integration via heat storage. In both Chapter 3 and Chapter 4, the models are applied to various examples. The conclusions are then summarised in Chapter 5 and recommendations for future work given. The relevant references follow each chapter and the Appendices appear at the end of this thesis.

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CHAPTER 2

LITERATURE REVIEW

2.1 Introduction

As the work in this thesis concerns batch processes, a background is given on batch scheduling. This includes various elements, such as the time horizon representation, flowsheet representation and operational philosophies. Various short-term scheduling techniques are then discussed. Long-term scheduling techniques then follow.

The main focus of this chapter, however, is incorporating heat integration into batch plant scheduling. Both direct and indirect heat integration are discussed. Examples are also given of how heat integration has been applied to energy intensive batch processes. Heat integration in continuous processes has not been included as this is well understood and is covered extensively in published literature.

A brief discussion of wastewater minimisation in batch plants as well as the combination of heat integration and wastewater minimisation is included, as this is relevant to the work in Chapter 3.

Finally, some conclusions are drawn highlighting the current state of scheduling, heat integration and combined heat integration and wastewater minimisation techniques in batch processes.

2.2 Operation of batch plants

Batch plants consist of unit operations occurring at distinct times during the time horizon, meaning processing units are not necessarily always active. A batch plant is classified as either multiproduct or multipurpose depending on how materials flow through the processing equipment (Sparrow *et al.*, 1975). Each batch of product follows the same equipment path in a multiproduct facility and production runs or campaigns are carried out for each product (Suhami & Mah, 1982). In a multipurpose plant, the batches can use different pieces of equipment and need not follow a single path. Multipurpose plants can be used to produce different products simultaneously or batches of the same product can also be produced at the same time while following completely different paths. Multipurpose plants are more flexible than multiproduct plants, but also more complex. Multiproduct plants are a subset of multipurpose plants and a mathematical model used to solve a multipurpose batch problem can also be used to solve the multiproduct case. The converse, however, is not true.

2.3 Operational philosophies

Scheduling considerations include the choice of flowsheet and time horizon representation as well as operational philosophies, which determine storage policies for intermediates and affect the flow of materials through units.

Operational philosophies relate intermediate product flows to available storage and units within the plant and a number of possibilities exist (Pattinson & Majozi, 2010).

UIS: Unlimited intermediate storage. Storage is guaranteed for intermediates after they have been produced. A unit becomes available to start processing the next batch as soon as the current batch has been completed.

NIS: No intermediate storage. An intermediate may have to be stored temporarily in the current processing unit, as dedicated intermediate storage elsewhere is unavailable. The material will only be transferred when the next unit becomes available, thus also freeing up the current unit for the next batch.

FIS: Finite intermediate storage. Storage available for intermediates is limited and can therefore not be guaranteed.

ZW: Zero wait. Intermediates must be transferred immediately after processing which means the next unit must be available. There is no intermediate storage available and the material may not be stored temporarily in the current processing unit. For example, this policy is important for unstable intermediates.

MIS: Mixed intermediate storage. This combines the use of UIS, NIS, FIS and ZW.

CIS: Common intermediate storage. A common intermediate storage vessel may be used by various units.

PIS: Process intermediate storage. Idle processing units may be used as temporary storage vessels.

2.4 Scheduling in batch processes

Time poses an additional constraint when production is done by means of batch processing rather than via continuous operations. Optimal scheduling of batch operations in a plant becomes very important for the plant to operate efficiently and economically.

Optimal scheduling in batch operations aims to determine an optimal sequence of tasks which use limited resources, such as raw materials, process units and storage. This is usually based on an economic objective, such as maximising profit or minimising makespan. For makespan minimisation, the production target is known and must be accomplished in the shortest possible time. For maximisation of throughput, the time horizon of interest is defined and the objective is to maximise the production over this period. The aim of optimal scheduling is to use resources more efficiently and to improve the productivity of a batch plant.

The ability to reschedule operations contributes to the flexibility of a batch plant. This is especially true when considering short-term scheduling. The feasibility of the rescheduling will, however, depend on the modifications required to achieve the new schedule. A plant may need to be rescheduled after changes in the market or government regulations. Application of process integration techniques may also require changes to the schedule. Many methods have been developed for the optimal scheduling of batch plants and are generally based on mathematical programming. Mathematical modelling and optimisation can take account of the time dimension more easily than graphical methods and operation-specific constraints and different objective functions can also be taken into account. Large problems, however, may lead to long processing times due to the mathematical structure of batch optimisation problems. Solution times often also increase for longer time horizons.

Two of the most important aspects to consider when modelling scheduling problems are the representation of the time horizon and the flowsheet.

2.5 Time horizon representation

The representation of the time horizon has an important effect on the structure of the mathematical model, especially in terms of the number of binary variables. Two methods are common when representing the time horizon of interest (Majozi & Zhu, 2001).

2.5.1 Uniformly discretised time horizon

The time horizon is divided into a finite number of intervals of equal length. The time points therefore have predefined locations. The beginning and end of a task can only take place at the boundaries of an interval. The accuracy increases with an increased number of intervals. Since a binary variable is assigned to each interval, this can lead to an explosive binary dimension and an overly large model which is difficult to solve. From Figure 2.1 it can be seen that there are too few intervals and the beginning and end times for tasks are not represented accurately.

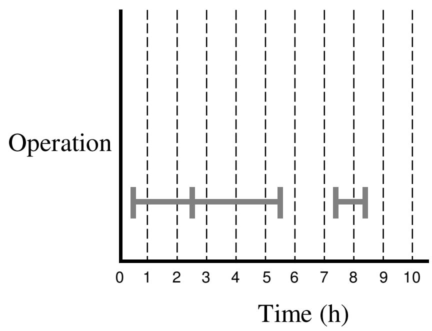

Figure 2.1. Tasks are not accurately represented.

If the number of intervals is increased, the situation in Figure 2.2 occurs. The tasks are represented accurately, but there are many unnecessary intervals, leading to unnecessary binary variables. For accuracy, the time horizon should be divided into intervals with a length which is equal to the highest common factor of the processing times.

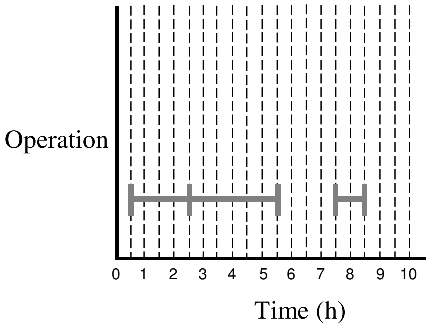

Figure 2.2. Tasks represented accurately, many unnecessary intervals.

2.5.2 Uneven discretisation of the time horizon

An uneven discretisation of the time horizon, or a continuous time based approach, solves the inherent limitation of the uniformly discretised time approach by allowing task events to take place at any point in time. This situation is shown in Figure 2.3. The time horizon is discretised into uneven time intervals with a specified number of time points, the locations of which are not prespecified. The boundaries of an interval denote the beginning or end of a task. Time points are allocated based on task durations and so the beginning and end times are represented accurately. There are also no unnecessary binary variables associated with unnecessary intervals.

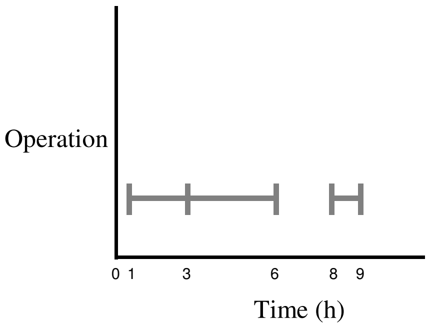

Figure 2.3. Uneven discretisation of the time horizon.

A drawback of the uneven discretisation of the time horizon is that the number of time points generally must be determined iteratively (Ierapetritou & Floudas, 1998; Shaik & Floudas, 2009). The recent model of Seid and Majozi (2012b), however, includes a method for accurately predicting the required number of time points.

Continuous time models may be classified into three categories: slot based, global event based and unit specific based formulations (Shaik *et al.*, 2006). Slot based methods represent the time horizon as ordered blocks of unknown, variable lengths or slots. Global event based models and unit specific event based models use continuous variables directly to represent the beginnings or endings of tasks. For global event based models, the set of events is common across all units. Unit specific event based models define events for each unit so tasks in different units may correspond to the same event point, but can occur at different absolute times. The unit specific event based representation is considered the most general and closest to true continuous time. When compared, the unit specific event based models are superior to slot based and global event based models in terms of the number of event points required to solve to global optimality.

Continuous time models are generally considered superior to discrete time models because they result in models with fewer time points and consequently fewer binary variables.

2.6 Flowsheet representation

The flowsheet is generally represented by the state task network (STN), resource task network (RTN) or more recently the state sequence network (SSN).

2.6.1 State task network (STN)

The STN was proposed by Kondili *et al.* (1993). The flowsheet is represented by three components. Circles represent states such as feeds, intermediates and products. Rectangles represent the tasks or operations that transform materials from input to output states by physical, chemical or biological means. Arcs connect the tasks with the states and define task precedence. An example of a STN for a simple sequential process is shown in Figure 2.4.

Figure 2.4. State task network (STN).

2.6.2 Resource task network (RTN)

The RTN was proposed by Pantelides (1994). The overall production facility is modelled as a collection of tasks and resources with some of the resources consumed and others formed. Similar to the STN, the representation uses two types of node, circles represent resources and rectangles represent tasks. The resources include feeds, intermediates, products, energy, manpower, storage and transportation facilities. The tasks are defined as for the STN, but also include transportation, cleaning and storage. An advantage of the RTN over the STN arises in problems involving identical equipment. Here the RTN formulation introduces a single binary variable instead of the multiple variables as used by the STN (Méndez *et al.*, 2006). The RTN representation for the same simple process is shown in Figure 2.5.

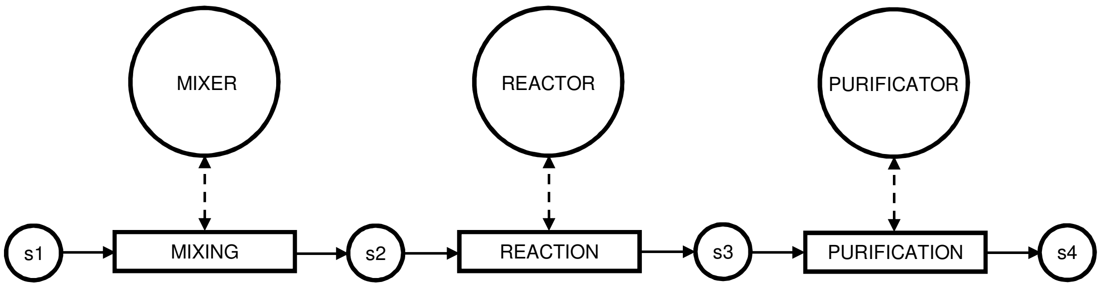

Figure 2.5. Resource task network (RTN).

2.6.3 State sequence network (SSN)

The SSN was developed by Majozi and Zhu (2001). This representation uses states only and tasks and units are implicitly incorporated. This dramatically reduces the number of binary variables in the formulation. If more than one state enters a unit, one of the states is chosen as the effective state. The total number of binary variables is then the number of effective states multiplied by the number of time points used. This further reduces the number of binary variables. The SSN also makes use of an uneven discretisation of the time horizon and the number of time points is determined iteratively. The SSN for the simple process is given in Figure 2.6.

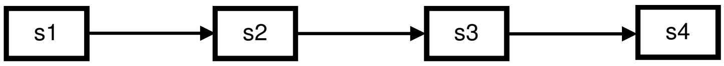

Figure 2.6. State sequence network (SSN).

2.7 Early mathematical methods for scheduling

The aim when solving the scheduling problem is to determine an optimal sequence of events in a batch process using the available resources. Most published techniques are based on mathematical programming with a resultant mixed integer linear programming (MILP) or mixed integer nonlinear programming (MINLP) formulation. The methods generally differ in the representation of the recipe and the time horizon.

A systematic formulation for the scheduling problem for multiproduct batch plants was proposed by Sparrow *et al.* (1975). Two methods were used to size the batch equipment. Firstly, the production requirements of each product were used to size the batch stages to achieve the required production. Secondly, a branch and bound technique was used to solve a MINLP problem to obtain a variety of feasible solutions with the objective of minimising equipment cost. A globally optimal solution, however, could not be guaranteed. Processing time for each batch was a function of the batch size and the overall run length of each product over the time horizon of interest depended on the number of batches processed.

Grossmann and Sargent (1979) formulated the scheduling problem as a geometric program. The Kuhn-Tucker conditions were used to prove that the resulting solution was globally optimal. When discrete equipment sizes were not included, the problem could also be solved as a relaxed subproblem.

Suhami and Mah (1982) formulated a MINLP problem for the optimal design of multipurpose batch plants with no intermediate storage. The objective was to minimise batch equipment cost. The model was solved using a generalised reduced gradient code. Batch sizes, time intervals, volumes of the reactors and the number of batch reactors were determined. The procedure yielded designs within 0.25% of the optimum.

Knopf *et al.* (1982) presented a general formulation for the optimisation of batch and semicontinuous plants. The objective was to minimise overall cost. Energy costs were also considered in the design optimisation. The formulation was a geometric program and was solved in the convexified primal form using a generalised reduced gradient code, OPT (Gabriele & Ragsdell, 1976).

Ravemark and Rippin (1998) applied the formulation of Sparrow *et al.* (1975) to multiproduct plants. A logarithmic transformation was used ensuring that the resulting model was convex. The objective was to minimise capital cost.

The methods proposed above were all limited to very small problems.

2.8 Short-term scheduling methods based on the STN

Kondili *et al.* (1993) proposed the state task network (STN) representation of a flowsheet, with circles representing states and rectangles representing tasks. The formulation was based on a uniformly discretised time horizon. This was a major drawback as it led to an explosive binary dimension, increasing the computational intensity required to solve the problem. Flexible equipment allocation, variable batch size and intermediate storage were also considered. Provision was made for raw materials available at the beginning or during the time horizon as well as for product deliveries during the time horizon. A three index binary variable was used to determine if unit *j* conducted task *i* at time point *p*. The resulting formulation was a MILP problem.

Shah *et al.* (1993a) extended the work of Kondili *et al.* (1993) aiming to reduce the computational requirement of the formulation. Various methods were used to do this, such as reformulation of constraints and derivation of a more compact linear programming relaxation of the MILP problem.

Mockus and Reklaitis (1997) presented a formulation, based on the STN representation and an uneven discretisation of the time horizon. The method could handle short-term scheduling problems in multiproduct or multipurpose batch plants. The scheduling problem was formulated as a MINLP which was then linearised to yield a mixed integer bilinear program (MIBLP). The model was solved using an outer approximation algorithm modified for nonconvexities. A global optimum was not found for the examples used. The model reduced to that of Kondili *et al*. (1993) if a uniform discretisation of the time horizon was used.

2.9 Short-term scheduling methods based on the RTN

Zhang (1995) and Zhang and Sargent (1996a), proposed a formulation based on the resource task network (RTN) representation and an uneven discretisation of the time horizon. The resultant mathematical formulation was a MINLP and was used to determine the optimal operating conditions of a mixed production facility. This model was linearised exactly using the Glover transformation (Glover, 1975), increasing the overall dimension of the problem and yielding a MILP.

The work of Zhang and Sargent (1996a) was later extended (Zhang & Sargent, 1996b) to handle operational constraints and plants involving continuous operations. Included was the concept of “unit usability” to incorporate various operational constraints such as task precedence and changeover. The usability would depend, for example, on the cleanliness of a unit.

A similar procedure based on the RTN representation was proposed by Schilling and Pantelides (1996). They used time points and time slots to represent the beginning and ending of tasks. Nonlinearities from the duration and resource balance constraints yielded a MINLP. These nonlinearities were linearised using the Glover transformation (Glover, 1975) and the resultant formulation was a MILP. Due to a large integrality gap as seen with formulations using an uneven discretisation of the time horizon, a novel branch and bound algorithm was used rather than the standard branch and bound techniques. This new technique used branching on both discrete and continuous variables. The integrality gap, however, remained large. The integrality gap is the difference between the solution of the integer problem (MILP) and the solution of the relaxed problem (LP).

The number of binary variables in the above STN and RTN formulations was i x j x p. This was due to the assignment of a single three index binary variable to describe when a task, i, occurred in a unit, j, at time point, p. This led to a large number of binary variables.

In order to decrease the number of binary variables, Ierapetritou and Floudas (1998) presented a new formulation based on the STN representation and an uneven discretisation of the time horizon. The time horizon was divided into event points which represented the beginning or end of a task at a point in the time horizon as well as the time between two event points. The optimal number of event points was determined iteratively. The most important feature of this formulation was a decoupling of units and tasks whereby separate binary variables were assigned to units and tasks. The number of binary variables in this case was (i + j) x p. This was less than or equal to the number obtained with the three index binary variable. The formulation was therefore well suited to large scale problems. The overall formulation was a MILP. The formulation had two major drawbacks, however. Firstly, the formulation initially predicted a large number of binary variables which was later reduced if there was one to one correspondence between units and tasks. Where a task took place in more than one unit or more than one task could take place in a unit, the number of binary variables could not be reduced. This reduction was also not always straightforward. Secondly, as is also true for the other formulations mentioned, the duration constraints were modelled as a function of batch size. This imposed restrictions on time and led to suboptimal results.

2.10 Short-term scheduling method based on the SSN

Majozi and Zhu (2001) developed a new representation for the process flowsheet, the state sequence network (SSN). In this representation, tasks were inferred and only states were considered. This eliminated the need for both task and unit binary variables, as required by the STN. Only one type of binary variable was used throughout the formulation. The binary variable associated with the usage of state *s* in unit *j* at time point *p* was $y(s_{in,j},p)$ and equalled one if state *s* was used in unit *j* at time point *p* and was zero otherwise. If more than one state entered a unit, only one input state needed to be defined and was an "effective state". The total number of binary variables was then the number of effective states multiplied by the number of time points used. This further reduced the number of binary variables. However, although a reduction in the number of binary variables is desirable, it does not always guarantee improved solution times (Sundaramoorthy & Karimi, 2005). The formulation was based on an uneven discretisation of the time horizon with time points denoting the beginning and ending of tasks. The result was a MILP problem which led to better results compared to previous formulations. The formulation also ensured an optimal schedule as outcome. Another novel idea presented was not modelling the duration constraints as a function of batch size, as done by previous authors. This was reflective of what actually happens in a batch process. The duration of a task is rather dependent on factors such as raw material purity, catalyst type and operator intervention. This approach led to much better results compared to modelling the duration constraints as a function of batch size, as the inherent time restriction was removed.

2.11 Short-term scheduling methods based on the S-Graph approach

Sanmartí *et al.* (1998) proposed a novel graph representation for scheduling the production of multipurpose batch plants. The method was flexible enough for a variety of production structures such as branches and alternative units. NIS and UIS transfer policies could be accommodated by choosing appropriate precedence relationships. The nodes of an S-Graph represented tasks and the arcs joining them represented the precedence relationships between them (recipe arc) and the order in which an equipment unit was used (schedule arc). The weight of an arc specified the processing time of the task corresponding to the initial node of the arc. If more than one equipment unit was available for this task, the weight of the arc was the minimum of the processing times of all possible equipment units. Extending the recipe graph in all directions resulted in all schedule graphs. A branch and bound procedure was used to generate the optimal schedule and the longest path algorithm was used to determine the minimum makespan. The S-Graph method did not require time points to be predefined, making it truly continuous in time. Problem specific characteristics could be incorporated into the solution algorithm improving computational efficiency. CPU time was also reduced with this method.

The S-Graph method was extended by Majozi and Friedler (2006) for maximisation of throughput or profit over a fixed time horizon. The optimisation procedure was based on a guided search algorithm that was guaranteed to terminate at a global optimum. Only the NIS operational policy was addressed. The formulation was applicable to fixed batch sizes, which occurs frequently in practice. The search region for *N* products was *N*-dimensional. Methods were discussed for reducing the search region which allowed the solution to be obtained much quicker than for an exhaustive search and quicker than the SSN.

2.12 More recent scheduling methods

Sundaramoorthy and Karimi (2005) proposed a synchronous or global event slot based, continuous time MILP formulation for short-term scheduling of multipurpose batch plants. Synchronous slots were used to simplify the treatment of shared resources, although this would require more slots compared to an asynchronous or unit specific event based method. Tasks were allowed to continue processing over multiple time slots which improved the results obtained. The formulation included no "Big M" constraints, which has been shown to improve MILP formulations. The model had fewer binary variables compared to formulations which decouple tasks and units. The number of time slots was, however, still increased in an iterative fashion. Rather than just inventory balances, the authors performed balances on processing times, resources and materials in processing units.

Shaik and Floudas (2009) presented a unit specific event based continuous time model based on the STN representation. The model was suitable for both batch and continuous plants and plants with or without shared resources. Tasks were allowed to take place over multiple event points. A three index binary variable was used to define when task i started at event n and ended at event n'. A parameter, Δn, was defined to control the maximum number of multiple events over which a task was allowed to continue. Apart from an iteration of the number of event points, for a given total number of events there was an additional iteration over Δn until a global optimal solution was found and the required CPU times were added over all the iterations.

Susarla *et al.* (2010) modified the model of Sundaramoorthy and Karimi (2005) and used unit specific slots instead of global slots. The model allowed non-simultaneous transfers of materials into or out of a batch, which resulted in better schedules. The authors highlighted the importance of constraint sequencing in GAMS for evaluating MILP based models as well as other factors such as the MILP solver, solver version, solver tuning options, "Big M" values and solution iterations. Tasks were allowed to span multiple slots and all units were forced to be empty at the end of the time horizon.

Seid and Majozi (2012a) presented a MILP formulation based on the state sequence network of Majozi and Zhu (2001) and unit specific time points. It had improved constraints for the proper sequencing of tasks and correctly handled the fixed intermediate storage (FIS) policy which had been violated in previous publications. The model resulted in a reduction of event or time points required and as a result, gave better performance in terms of objective value and CPU time required when compared to previous literature models. The formulation also included a method to predict the required number of time points using the concept of a critical unit and was shown to be very accurate (Seid & Majozi, 2012b).

2.13 Long-term scheduling methods

Wu and Ierapetritou (2004) presented a method for the cyclic scheduling of batch plants for scheduling over long time horizons. The assumption was that for a long time horizon and for the case where task durations are much shorter in comparison, there exists a sub-schedule with a shorter time horizon which, if repeated, may achieve an overall production close to the production achieved when periodic scheduling is not considered. It involves obtaining an optimal cyclic schedule which is then repeated and therefore reduces the problem size. It may also be easier to implement practically. This method was based on the previous discrete time model of Shah *et al*. (1993b) and rather used the continuous time scheduling constraints of Ierapetritou and Floudas (1998), based on the STN representation. It was assumed that the plant operated under stable conditions and would also have stable product requirements. The resulting model was a MINLP which was solved using both DICOPT and BARON. Cyclic scheduling sacrifices some accuracy when compared to the direct solution of the scheduling problem, but this is balanced by the easier solution of a less complex scheduling problem. The cyclic scheduling model was later rewritten for use with the SSN representation and was combined with wastewater minimisation constraints in order to minimise water usage over long time horizons in multipurpose batch plants (Nonyane & Majozi, 2012).

2.14 Heat integration in batch plants

Heating and cooling are unavoidable in many processing facilities, with operations where heat is generated and others where heat is required. It is because of this occurrence that heat integration becomes a possibility.

Heat integration in a batch process is complicated by the fact that it is constrained both by temperature and by time. Direct heat integration may be exploited when the heat source and heat sink processes are active over a common time interval. Alternately, indirect heat integration involves using a heat transfer fluid for storing energy and allows heat integration of processes regardless of the time interval. This is possible as long as the heat source process takes place before the heat sink process. This allows heat to be stored and then used later when required. The inclusion of heat storage instead of only direct heat integration leads to more flexibility in the process and therefore improved energy usage. In both cases, heat transfer may only take place if the thermal driving forces allow.

When applying heat integration to batch plants, there will be a trade-off between scheduling, savings achieved from heat integration, heat exchanger design and capital investment. After applying heat integration, the overall profit of a plant may increase due to savings from reduced utility consumption even though there may be a decrease in production or an increase in capital expenditure.

Methods for incorporating heat integration may either be sequential or simultaneous. Advantages and disadvantages exist for both (Halim & Srinivasan, 2009). Simultaneous consideration of scheduling and heat integration may lead to a more optimal solution. The problem may, however, become large for complex processes. For sequential methods, the model becomes simpler as it is split into two subproblems of scheduling and heat integration and can handle more complex problems. However, heat integration and batch scheduling are different types of optimisation problems with different objectives. The degree of heat integration depends on the production schedule. An optimal schedule could result in poor heat integration or optimal heat integration could lead to a poor scheduling solution (Adonyi *et al.*, 2003). Sequential problems, therefore, cannot be guaranteed to result in a global optimum.

2.15 Pinch analysis adapted for batch plants

Early techniques for heat integration in batch processes were based on pinch analysis, which was originally developed for heat integration in continuous plants at steady state. However, hot and cold streams in batch plants are not continuously available. Variations of the technique for batch processes still appear in literature. The major drawback of these techniques is their reliance on a predefined schedule, which leads to suboptimal results.

Kemp and Deakin (1989a) presented work on cascade analysis for heat integration in batch plants. Energy targets were set using the time average model (TAM) and time slice model (TSM). Time-temperature cascade tables determined the extent of heat recovery between streams via direct heat integration and heat recovery between different time intervals via heat storage. A three-dimensional cascade plot was also used to visualise heat flows. Kemp and Deakin (1989b) carried out heat exchanger network design using the energy targets from the cascade analysis. Methods for rescheduling to improve direct heat integration opportunities were explored and assessed. Kemp and Deakin (1989c) applied the cascade techniques to a case study based on a specialty chemicals plant and large savings could be achieved using direct heat integration and heat storage.

Pinch analysis using time dependent cascades was discussed by Kemp (1990). Stream heat loads could be averaged over a given batch cycle with targets obtained from the problem table, as for a continuous process. This was the pseudo-continuous or time average model (TAM). This model assumed all streams were continuously available and represented a limiting best case for the maximum heat recovery possible. To allow for the time factor, the time horizon for a single product plant using a predefined schedule was discretised into time intervals analogous to temperature intervals. All streams and materials were assumed to have steady state properties in each interval. Energy targets were calculated for direct heat exchange in each interval with a summation for the total energy target. Rescheduling was undertaken to increase the amount of heat directly exchanged, although no general method for this was discussed. Heat storage added an additional degree of freedom, but was considered secondary as it introduced additional expense in the form of a heat storage tank and an additional heat exchanger, which also reduced the temperature driving forces. Pinch analysis was shown to be applicable to total sites which could be modelled showing mean and peak loads.

Stoltze *et al.* (1995) proposed a method for waste heat recovery using only heat storage. A combinatorial method was used to determine an economically optimal number of heat storage units used. A search was performed among a set of feasible operating temperatures of heat storage units based on the supply and target temperatures of process streams. Utility added to heat storage units to restore their initial temperatures was accounted for; however, this led to wasted temperature driving forces. Costs taken into account to determine the economic optimum included those for tanks, pipes, pumps and heat exchangers. The authors found that the economics could be improved by adjusting storage temperatures, which decreased heat exchanger sizes.

Wang and Smith (1995) proposed a graphical method for heat integration based on pinch analysis, adapted for batch processes. The energy composite curve was plotted in the form of heat transferred versus time. Time was treated as the primary constraint, while temperature feasibility was treated as a secondary constraint. Both direct and indirect heat integration were considered. Opportunities for rescheduling were explored in order to decrease the heat storage requirement in favour of direct heat integration.

Instead of analysing batch streams from a thermodynamic perspective, Uhlenbruck *et al.* (2000) proposed first synthesising all possible heat exchanger networks using direct heat integration. A given schedule was divided into time and temperature intervals. Heating and cooling were assumed to take place at steady state within the time intervals, in order to apply pinch analysis. Heat cascades were used to identify hot and cold utility targets in each interval with the overall utility target obtained from summing those from each interval. One hot stream was allowed to exchange with one cold stream via a countercurrent heat exchanger. The heat recovery was improved further by matching with residual and previously unmatched streams. The method could not achieve the thermodynamic optimum.

Krummenacher and Favrat (2001) used a graphical pinch analysis technique for indirect heat integration in batch plants. The objective was to minimise the number of heat storage units required. The heat recovery range of the heat storage units was maximised by optimising their operating temperatures. Only indirect heat integration options were considered, even if there were opportunities for direct heat integration, such as overlapping hot and cold streams. This was under the assumption that direct heat integration could compromise the flexibility of the plant. Opportunities to reschedule streams in order to decrease heat storage capacity were evaluated. The possibility of reusing heat exchangers between streams with similar properties was also suggested. Preliminary mixed direct and indirect analysis was done only on a trial and error basis.

Problem table decomposition was extended from the continuous case for use in batch processes by Pourali *et al.* (2006). A predefined schedule was divided into time and temperature intervals. The time intervals were combined and pinch analysis was applied to target minimum energy requirements. A systematic combinatorial technique and the problem table algorithm were used for the analysis. The foundation for the method was that intervals, and therefore streams, may have better heat integration opportunities if combined. Heat storage possibilities were also considered. Different combinations were used, such as single streams, binary, ternary or higher, with rescheduling allowed to take place. The optimal solution was the one with maximum energy recovery and lower capital cost. A higher number of combinations in an interval introduced additional operational and process constraints making them less practical than combinations containing fewer streams. The number of possible combinations could be large which could make it difficult to find an optimal solution. However, the method was easily programmable.

Foo *et al*. (2008) presented a technique for targeting the minimum number of heat exchange units in a batch process, which was based on a similar technique developed for mass exchange networks (MEN) in batch plants. The method relied on a predefined schedule and determined a lower bound, whereafter the network was simplified. The minimum number of units was targeted above and below the pinch and in each time interval. Heat exchangers which shared intervals were reused if they connected the same hot and cold streams. The network could be further simplified by relaxing loops and the problem then became a trade-off between energy recovery and the number of heat exchangers. The consideration of heat storage in the network was also included and when applied to an oleic acid plant completely removed the need for cold utility.

Foo (2010) presented an automated targeting technique which could be used to target for batch heat exchanger networks (HEN), mass exchange networks (MEN) and water networks (WN). The mathematical optimisation model incorporated insight-based pinch analysis and was applied to fixed schedule problems. The schedule was divided into time intervals and targeting for the sources and sinks was performed for each interval with the overall target being the summation of the targets across all intervals. Inclusion of a storage system was used to improve heat or mass recovery.

Nemet *et al*. (2012) presented a technique for integrating solar thermal energy sources into processes with variable heat demands. A batch process heat integration method based on time slices and a piecewise-constant profile of heat availability was used. The use of heat storage also allowed heat to be transferred between heat slices, reducing the energy requirements by 42% in a case study. The case study was, however, based on a fixed schedule and rescheduling of the process was not considered. The method was also applicable to other renewable energy sources with fluctuating availability.

Chaturvedi and Bandyopadhyay (2014) presented an algorithm based on pinch analysis for targeting the minimum utility requirements for single and cyclic batch processes. The time horizon was divided into time intervals, each of which was then considered as a continuous process. The hot and cold utility requirements in each interval were then calculated using the problem table algorithm. Indirect heat integration between different time intervals via heat storage was also considered, although no design of the heat storage system was included. The method presented was, however, only applicable to batch processes with fixed schedules.

Wang *et al*. (2014) proposed a new heat integration method based on the heat duty versus time diagram, which could be applied to continuous plants featuring batch streams. The method combined the Gantt chart used in batch schedules and the temperature-enthalpy diagram used for heat integration of continuous plants. Both direct and indirect heat integration were considered as well as intra-batch and inter-batch heat integration. Both energy targets as well as heat exchanger network structures could be determined. A method was also given to optimise the network in terms of capital cost by removing units. The method was intuitive and could be applied methodically; however, it relied on a predefined schedule, as is the case with other methods based on pinch analysis.

Anastasovski (2014) presented a seven step method for the design of a common heat exchanger network for a plant producing yeast and alcohol, which included batch streams.

The time slice model (TSM) was used and heat exchanger networks were designed using the principles of pinch technology. A common heat exchanger network is one which can satisfy the heating and cooling requirements for each time slice and for each existing pair of streams in order to improve energy efficiency. The method used a previously optimised fixed schedule. Streams using a common heat exchanger were required to be compatible. If this was not the case, washing of the heat exchanger would have to be carried out. Heat exchanger splits were allowed so as to accommodate the use of the heat exchangers between different streams in different periods. The aim of this versatile use of heat exchangers was to minimise the heat loads and heat transfer area of the heat exchangers.

2.16 Mathematical techniques using a predefined schedule

For many mathematical heat integration techniques presented in published literature, the processing schedule also tends to be predefined, leading to suboptimal results. Some methods may include heuristic approaches which also cannot guarantee optimality.

Early work on heat integration in batch processes (Vaselenak *et al.*, 1986) explored heat exchange between hot and cold vessels requiring cooling and heating, respectively. The work addressed the problem of determining the maximum heat integration possible, to reduce consumption of external utilities. A MILP formulation was used when temperatures were limiting and heuristics were used when temperatures were not limiting. The fluids themselves were either transferred or a heat transfer medium was used to transfer heat. Process fluids were either returned to their starting vessels or transferred to receiving vessels. In the analysis, a batch could not be split, therefore only one to one matches were allowed.

Ivanov *et al.* (1993a; 1993b; 1993c) considered heat integration between a hot reactor and a cold reactor, active at different times. Indirect heat integration using either two heat storage tanks or one combined heat storage tank was considered. Three different arrangements were used for each case and mathematical models were developed describing the variations in temperature of the vessels with time. The three cases analysed were: both streams recycled; one stream recycled or both streams transferred to receiving tanks. The result was a mathematical model for cyclic cooling and heating for a reactor system. Two heat storage tanks were used for the case where the number of hot and cold vessels was equal (Ivanov *et al.*, 1993a) – one hot storage tank and one cold storage tank. Flowrates of streams were assumed constant and transient processes in the vessels were not considered. Also, heat losses were assumed negligible.

Mathematical expressions for temperature variations with time were also developed for the case of one combined heat storage unit (Ivanov *et al.*, 1993b). This was applicable when the number of hot and cold streams was not equal. The possibility for direct heat integration when streams occurred simultaneously was also considered.

Ivanov *et al.* (1993c) used the results from Ivanov *et al.* (1993a) and Ivanov *et al.* (1993b) for synthesising new heat integrated plants and reconstructing existing ones using heat storage tanks for maximising energy recovery. For the reconstruction of existing chemical plants, it was assumed the existing external utility systems would remain unchanged. The problems obtained were nonlinear and were solved using the method of adaptive nonlinear optimisation.

Corominas *et al.* (1993) proposed a method for plants running in campaign mode. The objective was to design an optimal heat exchanger network with minimum energy consumption for each campaign. The networks of all campaigns were also grouped into a single macronetwork containing matches common to different campaigns. Only one to one matches were considered and no heat storage possibilities were explored. All possible combinations between hot and cold streams were generated and one pair was selected based on highest energy requirements. The relative timing of the tasks was altered if necessary to find simultaneous streams. A common heat exchanger unit could be used if two products had similar chemical properties, such as viscosity, heat capacity and flowrate, however, this would lead to increased cleaning requirements.

Vaklieva-Bancheva *et al.* (1996) considered direct heat integration with the objective of minimising total costs. The nonlinear objective function was linearised with additional variables and constraints and the resulting overall formulation was a MILP, solved to global optimality. Zero-wait fixed the relative timing of all stages and the method was suitable for existing plants with a fixed set of processing equipment. The method was restricted to one to one matches and only specific pairs of units were allowed to undergo heat integration.

Bozan *et al.* (2001) presented a two part approach for optimising the cost of a heat exchange network for direct heat integration. Product campaigns were determined using a heuristic procedure to specify the locations of heat exchangers. Heat exchange areas for the possible heat exchangers were then found by solving a nonlinear optimisation model with a grid search algorithm. The minimum total cost heat exchanger network optimisation was then modelled as a MILP modified from Vaklieva-Bancheva *et al.* (1996) and included the operating costs of hot and cold utilities and the annualised capital costs of heat exchange units. This solution resulted in a large number of near optimal solutions which could be practically applied. Sensitivity analysis was done considering hot and cold utility processes. Heat integration was favoured if the prices of hot and cold utilities were high. If they were low, unintegrated processing was favoured to avoid heat exchanger capital costs.

De Boer *et al.* (2006) investigated an industrial heat storage system within an existing production facility. Three different thermal storage systems were designed to store the heat released during an exothermic reaction phase and reuse the heat for preheating the reactants in the following batch. Savings between 50% and 70% could be achieved; however, payback time was greater than 10 years. Direct heat integration from a hot batch to the next cold batch was not practical because of process control difficulties.

Chen and Ciou (2008) also considered using only indirect heat integration and solved a MINLP formulation using a global solver. Multiple heat storage vessels could be used, but additional vessels did not guarantee improved heat recovery efficiency.

Halim and Srinivasan (2008) proposed a multi-objective method using direct heat integration with cocurrent heat exchange. It was, however, presented as a simultaneous method. The mathematical model was based on the STN continuous time synchronised slot based MILP formulation of Sundaramoorthy and Karimi (2005). The objective was to minimise makespan. A number of optimal schedules were found and heat integration using the TAM and TSM was performed on each (Kemp, 1990). The schedule requiring the least utilities was chosen as the best. Scheduling and heat integration were therefore performed sequentially rather than simultaneously. The method was later cited as sequential rather than simultaneous (Halim and Srinivasan, 2009) and schedules were optimised in terms of minimum makespan or maximum profit, while minimising utilities. It was argued that sequential procedures could lead to a higher number of practically implementable networks with an optimal schedule and could also be more suitable for complex problems. Non-optimal schedules were also analysed for heat integration to allow for possible trade-offs between schedules and utilities.

Al-Mutairi and El-Halwagi (2009) presented a procedure to incorporate direct heat integration and process scheduling into a continuous plant with schedules varying due to changes in demand. Temperatures and flowrates were allowed to vary within given upper and lower bounds. The process was, however, assumed to operate at steady state for each anticipated schedule. Storage of heat to be used in another scheduling period was not considered. A single heat exchanger network was designed to accommodate all expected variations of the schedule.

The main advantage of the sequential approaches is their ability to solve the heat integration problem without many of the assumptions necessary for simultaneous methods. However, they usually result in suboptimal solutions (Halim & Srinivasan, 2009).

2.17 Simultaneous scheduling and heat integration approaches

Methods dependent on a predefined schedule or where energy requirements are averaged over time intervals lead to suboptimal results. Methods which capture the essence of time and are specifically applicable to batch plants are therefore required. For a more optimal solution, scheduling and heat integration may be combined into a single problem. However, models may then need to be simplified in order to avoid excessive solution times.

Papageorgiou *et al.* (1994) embedded a heat integration model within the scheduling formulation of Kondili *et al.* (1993). Opportunities for both direct and indirect heat integration were considered as well as possible heat losses from the heat storage tank. Differential equations were integrated numerically over the discrete time horizon. However, discretisation of the time horizon always leads to an explosive binary dimension. The resulting model was a nonconvex MINLP, for which a global optimum could not be guaranteed. The operating policy in terms of heat integrated or standalone was also predefined for tasks. This work was extended by Georgiadis and Papageorgiou (2001) to consider fouling of heat exchange units and the associated cleaning schedules and costs. It was found that fouling can significantly affect a production schedule as well as heat integration opportunities.

Lee and Reklaitis (1995a) presented a method for scheduling with maximum energy recovery from direct heat integration in cyclically operated processes producing a single product. Only one to one matches were considered, as multiple matches would require a more complex formulation without guaranteeing better results. Heat exchange time was assumed negligible compared to batch processing time as this depends on the flowrates of the fluids, area of the heat exchanger and the minimum approach temperature for heat exchange. These are usually chosen considering a trade-off between time and the cost of the heat exchangers. Streams were considered available only when a fluid was transferred from one unit to the next and transfer times were scheduled such that pairs of streams could coexist. Utility savings showed an increase with increased allowable holding times. The formulation was extended (Lee & Reklaitis, 1995b) to include finite exchange times. Shared heat exchange units across multiple matches were considered to minimise the number of heat exchange units. This, however, led to complex mixed integer nonlinear constraints.

Zhao *et al.* (1998a) removed the restriction of one to one matches, allowing multiple stream matching within the same period of time using heat cascade analysis. Countercurrent heat exchange was used due to its inherently higher thermodynamic efficiency. The resultant formulation was a MINLP which was solved using NLP and MILP subproblems and was only suitable for small problems. A simplification of constant heat exchange time between streams led to a MILP formulation. Rescheduling was included so more streams could coexist for direct heat integration (Kemp, 1990).

Zhao *et al.* (1998b) also proposed a three step design procedure for designing heat exchanger networks. The problem was decomposed into three simpler subproblems: an initial individual design, rematching design and final overall design. This method was, however, based on a predefined schedule. In the first stage, techniques and heuristic procedures used for continuous processes were used to design the heat exchanger network for each time interval, but designs in each interval could not easily be combined to give a good design for the whole system. For the second stage, a MILP model was used to adjust matched streams, aiming at maximum use of common heat exchangers in order to reduce energy and capital costs. The third stage involved a search for opportunities for further trade-off between energy and capital to get a final cost effective design using heuristics. A globally optimal solution could not be guaranteed.

Pinto *et al.* (2003) presented a MILP formulation for direct heat integration with the objective of optimising the plant in terms of revenue, operating costs and capital expenditure. Only one to one matches were considered. A discrete time representation of the time horizon was used, which resulted in a large number of binary variables.

Adonyi *et al.* (2003) used the "S-Graph" scheduling approach (Sanmartí *et al.*, 1998) and incorporated one to one direct heat integration. Heat integration was greatly improved with a small compromise in minimal makespan.

Majozi (2006) presented a direct heat integration formulation based on the SSN recipe representation and an unevenly discretised time horizon (Majozi & Zhu, 2001). This model used fewer binary variables compared to previous formulations based on the STN. The model considered both fixed and variable batch sizes. The formulation as given was, however, more suited to multiproduct applications rather than multipurpose facilities. This work was later extended (Majozi, 2009) to include heat storage for indirect heat integration. The heat storage capacity and the initial heat storage temperature were, however, predefined parameters. Although this led to a MILP problem, suboptimal results were obtained. This model was also for multiproduct facilities.

Chen and Chang (2009) extended the work of Majozi (2006) to periodic scheduling with direct heat integration, based on the RTN. The resultant direct heat integration formulation was a MILP. The SSN representation (Majozi, 2006) used fewer binary variables than the RTN approach for the heat integrated short-term scheduling case, while achieving the same objective value. However, for the periodic case, all heat sources and sinks operated in integrated mode making the process more economical.

Stamp and Majozi (2011) presented a simultaneous scheduling and heat integration formulation suitable for multipurpose batch plants based on the work of Majozi (2009). This model optimised the initial heat storage temperature as well as the heat storage capacity.

Heat losses from the heat storage vessel were also considered and were found to be negligible. The model forms the basis of the work in this thesis.

The review on heat integration in batch plants by Fernández *et al.* (2012) provides an overview of both older and more recent heat integration methods.

Seid and Majozi (2014a) presented a simultaneous model where the heat integration constraints were embedded in the recent scheduling formulation of Seid and Majozi (2012a). This scheduling model has proven to lead to better results in terms of fewer required time points and therefore reduced computational time as well as better objective values. The model also provides for the correct sequencing of tasks for the FIS policy. Both direct and indirect heat integration were considered as well as either fixed or variable batch sizes. A task could also be heat integrated with other tasks in more than one time interval to improve heat recovery. Also, the model allowed a task to integrate with another task during any interval between the starting and finishing time of the task. The time average model (TAM) was used whereby heat flows were averaged over the processing times of the tasks.

Lee *et al.* (2015) presented a mathematical technique for multipurpose batch plants where, instead of heating and cooling *in situ*, hot and cold stream pairs with feasible temperature driving forces underwent heat integration during material transfer from one unit to the next. The proposed model optimised the coincidence of these stream pairs. This method of heating and cooling also reduced the time required for processing and results from a case study showed improvements of more than 30% in energy savings and 15% in product throughput due to time savings.

2.18 Specific heat integration applications

Energy intensive noncontinuous processes are common in the food, beverage, biochemical and agrochemical industries. Within the food industry, the dairy and slaughtering and meat processing industries have high electricity demands. The sugar industry and drink production plants on the other hand are particularly fuel demanding (Fritzson & Berntsson, 2006). Scheduling and heat integration of these plants is complicated due to low and varying production volumes as well as recipes which vary with time and demand. Operating hours per year can also be rather low.

Knopf *et al.* (1982) analysed a noncontinuous cottage cheese process and concluded that capital costs were far outweighed by the energy costs in the plant.

Boyadjiev *et al.* (1996) applied a sequential analysis for direct heat integration in an existing antibiotics plant. The effluent cooling water was used as makeup for the hot water. This simultaneously reduced the overall energy cost, freshwater consumption and waste, in the form of warm water. Energy costs for the plant decreased by 39%.

Atkins *et al.* (2010) investigated heat integration in a milk powder processing plant. Both intraplant as well as interplant integration were considered. Direct heat integration was favoured for intraplant heat integration while indirect heat integration using one thermally stratified tank was favoured for interplant heat integration. Thermal storage was important in such a process because there were fewer heat sinks than heat sources available. The effect of the hot temperature in the heat storage tank on the maximum heat recovery potential was investigated. A predefined schedule was used with known profiles for heat sources and heat sinks.

Tokos *et al.* (2010) investigated retrofit heat integration in the brewhouse of a brewery. The mathematical model was based on the work of Lee and Reklaitis (1995a) for single product batch plants having no intermediate storage. Heat integration was considered over multiple batches. Integration of a unit with more than one other unit was allowed with the ending time of the first equal to the starting time of the second. Utility savings were traded off against heat exchanger investment costs. It was concluded that there was already a high level of heat integration achieved in the brewhouse, while there may be opportunities for additional savings when including the total site, such as the packaging line.

Rašković *et al.* (2010) identified an opportunity for significant waste heat recovery in a yeast and ethanol production plant, even though such a plant is not usually considered energy intensive. Although production was semi-continuous, during certain times the subsystems with streams involved in heat recovery operated simultaneously. This simplification was made in order to apply pinch analysis.

Fritzson and Berntsson (2006) applied heat integration to a slaughter and meat processing plant. The plant already had a modern heat recovery system in place, but savings of 30% of the external heat demand and 10% of the shaftwork used in the plant could still be achieved.

Majozi (2009) combined both direct and indirect heat integration with scheduling and applied the model to an agrochemical facility. Savings of more than 75% in external steam consumption in the plant were achieved. Optimisation of the heat storage capacity and initial heat storage temperature further reduced the requirement for external steam by 33% compared to using known parameters (Stamp & Majozi, 2011).

2.19 Heat storage

Introducing heat storage can increase the chances of finding heat integration matches and improve the performance and availability of energy sources and sinks. However, the benefits depend largely on cost and an economic analysis is important to decide whether to incorporate heat storage or not (Zhihong & Hua, 2003).

Including a heat storage system in an existing facility becomes a large part of the total cost. The capital costs of an indirect heat exchanger network include the area of the heat exchangers, a heat storage vessel and the fixed costs of the heat exchangers, for example piping. Using indirect heat integration, two heat exchangers are required and temperature driving forces are split between them. With direct heat integration only one heat exchanger is required and a heat storage vessel is not necessary (Kemp, 1990). Methods for simplifying heat exchanger networks become important, such as eliminating small, uneconomic heat exchangers. It is more beneficial to evaluate using heat storage systems in new designs (De Boer *et al.*, 2006) and the heat storage system should have a high rate of use to be more economical.

Heat exchange via a heat storage medium may be by temperature difference using the sensible heat of the substance or using constant temperature, for example with thermowells or latent heat (Kemp, 1990). Selection factors to consider when choosing a heat storage medium include a wide temperature range to maintain liquid phase, high heat capacity, high density, low volatility and low corrosiveness (Chen & Ciou, 2008). Heat storage materials should also be low in cost and have a high thermal conductivity. It is also important to reduce heat losses through insulation (Caruso *et al.*, 1989).

2.20 Wastewater minimisation in batch plants

In multipurpose batch plants, after completing a task a shared unit is required to be washed before performing subsequent tasks. Equipment cleaning is usually associated with large amounts of water and these washing operations present an opportunity for wastewater minimisation. Efficient use of water is essential for ensuring that the amount of freshwater consumed as well as the amount of wastewater generated are minimised. Water from a unit can be recycled into the same unit, reused by other units or sent to a water storage vessel. Direct water reuse refers to the use of an outlet wastewater stream from one unit into another unit, while indirect water reuse refers to the use of previously stored wastewater into a unit. A wastewater regenerator can also be used to purify wastewater to a quality where it can be reused in other operations, further increasing water reuse opportunities.

As heat integration is the main focus of this thesis and wastewater minimisation a secondary consideration, only a few recent publications are discussed.

Majozi and Gouws (2009) presented a model for wastewater minimisation in multipurpose batch plants with multiple contaminants. The water usage and schedule were optimised simultaneously and the use of a central reusable water storage unit was investigated.

Adekola and Majozi (2011) extended the multiple contaminant model of Majozi and Gouws (2009) and included a regeneration unit. A regenerator is used to purify water in the plant and as such improves the opportunities for wastewater reuse. Water was transferred to the regenerator if a unit required water with a contaminant concentration lower than that which was available from either central storage or from other units. It therefore only operated intermittently.

Nonyane and Majozi (2012) presented a long-term wastewater minimisation technique in which wastewater minimisation constraints were combined with the long-term, cyclic scheduling model of Wu and Ierapetritou (2004). Whereas most wastewater minimisation methods published in literature are based on short-term scheduling techniques, this model could be applied over longer time horizons. As time was treated as a variable, production as well as water usage could be optimised simultaneously. The model also considered the start-up and shut-down phases of operation. Water was minimised using opportunities for reuse and recycle and the possibility of using a central water storage unit was included.

2.21 Combined heat integration and wastewater minimisation

The combined consideration of wastewater minimisation and heat integration in batch plants has been largely ignored, due to the potential complexities of such a problem. This problem has been addressed in continuous processes, using graphical methods (Savulescu *et al.*, 2005; Wan Alwi *et al.*, 2011) and mathematical optimisation (Dong *et al.*, 2008;

Leewongtanawit & Kim, 2008; Kim *et al.*, 2009; Sahu & Bandyopadhyay, 2012; Chew *et al.*, 2013).

Halim and Srinivasan (2011) developed a framework for multipurpose batch plants that integrated scheduling, direct heat integration and direct water reuse optimisation based on a sequential technique. Firstly, the process schedule was optimised to meet an economic objective. This was followed by the generation of alternate schedules through a stochastic search-based integer cut procedure. Next, heat integration analysis and water reuse synthesis were each performed to optimise energy and water requirements on each schedule. Although the aim was to retain the optimality of the scheduling solution, a sequential technique cannot guarantee an overall optimal result.

Adekola *et al*. (2013) presented a model for the simultaneous optimisation of both energy and water within a flexible scheduling framework for multipurpose batch plants. A flexible process schedule can give an improved result in the form of a better overall production schedule compared to schedules obtained from optimising energy and water separately. The model was a combination of the scheduling framework of Majozi and Zhu (2001), the heat integration model of Stamp and Majozi (2011) and the wastewater minimisation model of Adekola and Majozi (2011). With respect to energy optimisation, both direct and indirect heat integration were explored for reducing external utility requirements. With respect to wastewater minimisation, opportunities for direct water reuse and indirect water reuse utilising wastewater storage were explored. The objective was to improve the profitability of the plant by minimising external utility usage and wastewater generation. This work is presented in full in Chapter 3 of this thesis.

Seid and Majozi (2014b) presented a model for combined energy and water minimisation in multipurpose batch plants. The scheduling model of Seid and Majozi (2012a) was used and combined with heat integration and wastewater minimisation constraints. The model allowed simultaneous optimisation of scheduling as well as energy and water use. The time average model (TAM) and time slice model (TSM) were used. However, the time slices were variables determined by optimisation. Heat integrating units were not forced to start simultaneously, but were allowed to integrate any time between the starting and finishing time of the task, which improved the flexibility of the schedule. Tasks could also be heat integrated with other tasks in more than one time interval. The model only allowed for direct heat integration and direct reuse of water.

2.22 Conclusions

The productivity and revenue of a plant can be enhanced by proper scheduling, especially in multipurpose batch plants. Various methods exist and differ mainly with regards to the representation of the flowsheet and the time horizon of interest. The SSN formulation of Majozi and Zhu (2001) has proven to reduce the number of binary variables, which as a rule of thumb reduces computational time. The method of Seid and Majozi (2012a) is also based on the SSN and has shown to result in better objective functions, fewer required time points and reduced computational time.

Batch plants are generally run on a smaller scale compared to continuous processes and require lower utilities; however, certain batch industries are energy intensive. Due to the increasing popularity of batch plants, energy efficiency can no longer be ignored.

Early heat integration techniques are based on techniques originally developed for continuous processes, such as pinch analysis. These techniques are unable to capture the essence of time in a batch process and are therefore insufficient for exploring heat integration possibilities.

Most heat integration methods for batch plants discussed in published literature either rely on a predefined schedule or consider only one type of heat integration, i.e. direct or indirect. Both lead to suboptimal results. However, simultaneous models may become large for more complex problems. Combining both direct and indirect heat integration may also lead to increased costs and complexity.

Using both direct heat integration and indirect heat integration via heat storage may significantly reduce utility needs in a batch processing plant. This is due to an increase in flexibility in the process, since heat sources and heat sinks need not be active over a common time interval in order to explore heat integration opportunities.

When using heat storage for indirect heat integration, an additional heat exchanger is required for the match, compared to the case of direct heat integration. For heat storage to be economical, it must be used frequently with low storage times between batches to decrease heat losses from the heat storage tank. Good insulation on the heat storage vessel must also be maintained.

Washing of shared units becomes essential in multipurpose batch plants after a task has been completed and this requires large quantities of water. The amount of freshwater used and wastewater generated can be minimised using recycle and reuse.

Current long-term heat integration methods have only been applied to multiproduct batch plants and do not include the use of heat storage. However, a technique does exist in literature for long-term wastewater minimisation in multipurpose batch plants.

A sequential method exists for combined energy and wastewater minimisation in multipurpose batch plants (Halim & Srinivasan, 2011). However, a sequential approach is not guaranteed to lead to an optimal solution. Two more recent methods have been published and the method of Adekola *et al*. (2013) is presented in full in the next chapter.

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CHAPTER 3

SIMULTANEOUS ENERGY AND WATER OPTIMISATION

3.1 Introduction

Minimising energy usage and water consumption is influenced by the need to abide by stricter environmental regulations, reduce the effects of higher energy prices and conserve scarce environmental resources. In this chapter, the heat integration model of Stamp and Majozi (2011) has been extended to include wastewater minimisation constraints from the model of Adekola and Majozi (2011). A combined model is therefore presented for the simultaneous optimisation of both energy and water usage within a flexible scheduling framework for multipurpose batch plants. A flexible process schedule can give an improved result in the form of a better overall production schedule compared to schedules obtained from optimising energy and water separately. With respect to energy optimisation, both direct and indirect heat integration are explored, with the aim of reducing external utility requirements. With respect to wastewater minimisation, opportunities for direct water reuse and indirect water reuse utilising wastewater storage are explored. The objective is to improve the profitability of the plant by minimising both utility usage and wastewater generation. The results from three examples are presented. The work presented in this chapter has also recently been published (Adekola *et al*., 2013).

3.2 Problem statement and objective

The problem addressed in this chapter involves the optimisation of energy and water within a production scheduling framework. In production scheduling, the objective is either profit maximisation or minimisation of makespan. During production, certain tasks require cooling or heating, for instance, exothermic reactions that require cooling or endothermic reactions that require heating. The requirements for heating or cooling afford opportunities for heat integration. In multipurpose batch plants, particularly at the completion of a processing task in a unit, the equipment unit is washed before performing subsequent tasks. This is to ensure product integrity through prevention of contamination. The washing operations present the opportunity for wastewater minimisation. It is assumed that no heat or water losses occur.

The problem can be stated formally as follows:

Given:

Scheduling data

(i) production recipe for each product

(ii) available units and their capacities

(iii) maximum storage capacity for each material

(iv) task durations

(v) time horizon of interest or predetermined production

(vi) costs of raw materials

(vii) selling price of final products

Heat integration data

(i) hot duties for tasks requiring heating and cold duties for tasks that require cooling

(ii) operating temperatures of heat sources and heat sinks

(iii) minimum allowable temperature differences

(iv) heat capacities of materials

(v) costs of hot and cold utilities

(vi) design limits on heat storage

Wastewater minimisation data

(i) washing time for each unit

(ii) mass load of contaminants in each unit

(iii) maximum inlet and outlet concentrations of contaminants for each unit

(iv) maximum storage available for water reuse

(v) cost of freshwater

(vi) cost of effluent treatment

The objective is then to determine an optimal production schedule that achieves a maximum profit or minimum makespan, requiring the minimum amount of external utilities and freshwater use.

3.3 Mathematical model

The mathematical formulation consists of the three modules given in the problem statement, i.e. the production scheduling, heat integration and wastewater minimisation modules. The necessary heat integration and wastewater minimisation constraints are embedded in the scheduling framework. The model uses the scheduling framework of Majozi and Zhu (2001), which features the state sequence network (SSN) recipe representation and an uneven discretisation of the time horizon. This scheduling framework has proven to result in fewer binary variables compared to models based on other representations. The constraints of the scheduling formulation may be found in Appendix A. The heat integration constraints of Stamp and Majozi (2011) are presented first, followed by the necessary wastewater minimisation constraints of Adekola and Majozi (2011). The mathematical model is based on the superstructures in Figure 3.1. Figure 3.1(a) is the superstructure for heat integration while Figure 3.1(b) is the superstructure for water optimisation.

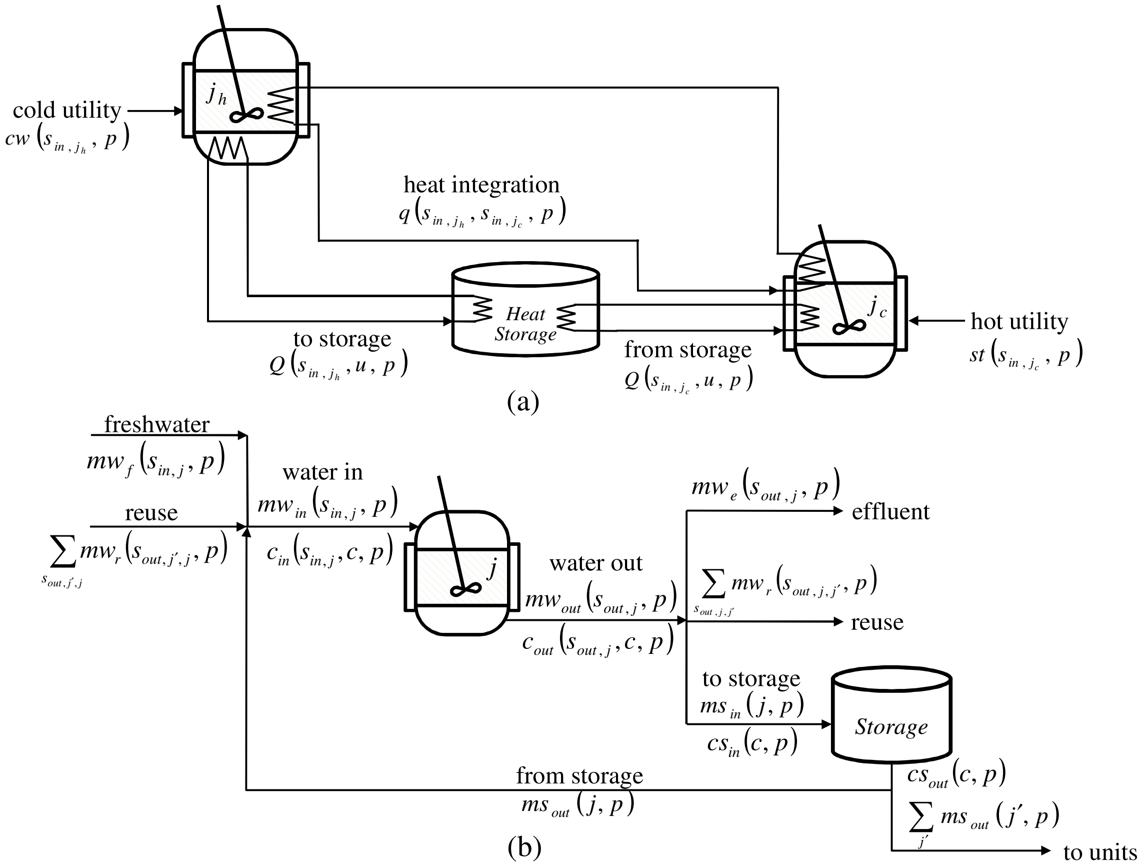

Figure 3.1. Superstructure for mathematical formulation: (a) when units perform heating/cooling tasks, (b) when units perform washing tasks.

Heat integration constraints

The heat integration constraints are based on the superstructure in Figure 3.1(a). Each processing unit may operate using either direct or indirect heat integration. Direct heat integration refers to the use of heat generated from a processing unit to supply a processing unit requiring heat, without the use of heat storage. Indirect heat integration refers to the use of heat previously stored in a heat storage vessel to supply a processing unit requiring heat. The heat is stored through a heat transfer fluid medium, e.g. water. Processing units may also operate in standalone mode, using only external utilities. This may be required for control reasons or when thermal driving forces or time do not allow for heat integration. If either direct or indirect heat integration is not sufficient to satisfy the required duty, external utilities may make up for any deficit.

Constraints (3.1) to (3.39) constitute the heat integration model, useful for multipurpose batch processes. The formulation is based on the model of Stamp and Majozi (2011) and includes direct and indirect heat integration.

Constraints (3.1) and (3.2) are active simultaneously and ensure that one hot unit will be integrated with one cold unit when direct heat integration takes place, in order to simplify operation of the process. Also, if two units are to be heat integrated at a given time point, they must both be active at that time point. However, if a unit is active, it may operate in either integrated or standalone mode.

$$\sum_{s_{in,j_c}} x\left(s_{in,j_c}, s_{in,j_h}, p\right) \leq y\left(s_{in,j_h}, p\right), \qquad \forall\ p \in P,\quad s_{in,j_h} \in S_{in,j} \tag{3.1}$$

$$\sum_{s_{in,j_h}} x\left(s_{in,j_c}, s_{in,j_h}, p\right) \leq y\left(s_{in,j_c}, p\right), \qquad \forall\ p \in P,\quad s_{in,j_c} \in S_{in,j} \tag{3.2}$$

Constraints (3.3) and (3.4) ensure that heat integration between a unit and heat storage may occur only if the unit is active at that time point. However, if a unit is active, it will not necessarily integrate with heat storage.

$$z\left(s_{in,j_c}, u, p\right) \leq y\left(s_{in,j_c}, p\right), \qquad \forall\ p \in P,\quad s_{in,j_c} \in S_{in,j},\quad u \in U \tag{3.3}$$

$$z\left(s_{in,j_h}, u, p\right) \leq y\left(s_{in,j_h}, p\right), \qquad \forall\ p \in P,\quad s_{in,j_h} \in S_{in,j},\quad u \in U \tag{3.4}$$

Constraint (3.5) ensures that heat storage is heat integrated with either one hot unit or one cold unit at any point in time. This is to simplify and improve operational efficiency in the plant.

$$\sum_{s_{in,j_c}} z\left(s_{in,j_c}, u, p\right) + \sum_{s_{in,j_h}} z\left(s_{in,j_h}, u, p\right) \leq 1, \qquad \forall\, p \in P,\ \ u \in U \tag{3.5}$$

Constraints (3.6) and (3.7) ensure that a unit cannot simultaneously undergo direct and indirect heat integration. This condition simplifies the operation of the process.

$$\sum_{s_{in,j_h}} x\left(s_{in,j_c}, s_{in,j_h}, p\right) + z\left(s_{in,j_c}, u, p\right) \leq 1, \qquad \forall\, p \in P,\ \ s_{in,j_c} \in S_{in,j},\ \ u \in U \tag{3.6}$$

$$\sum_{s_{in,j_c}} x\left(s_{in,j_c}, s_{in,j_h}, p\right) + z\left(s_{in,j_h}, u, p\right) \leq 1, \qquad \forall\, p \in P,\ \ s_{in,j_h} \in S_{in,j},\ \ u \in U \tag{3.7}$$

Constraints (3.8) and (3.9) quantify the amount of heat received from or transferred to the heat storage unit, respectively. There will be no heat received or transferred if the binary variable signifying use of the heat storage vessel, $z\left(s_{in,j}, u, p\right)$, is zero. These constraints are active over the entire time horizon, where p is the current time point and $p-1$ is the previous time point.

$$Q\left(s_{in,j_c}, u, p-1\right) = W(u)\, cp_{fluid}\left(T_0(u, p-1) - T_f(u, p)\right) z\left(s_{in,j_c}, u, p-1\right),$$
$$\forall\, p \in P, p > p0,\ \ s_{in,j_c} \in S_{in,j},\ \ u \in U \tag{3.8}$$

$$Q\left(s_{in,j_h}, u, p-1\right) = W(u)\, cp_{fluid}\left(T_f(u, p) - T_0(u, p-1)\right) z\left(s_{in,j_h}, u, p-1\right),$$
$$\forall\, p \in P, p > p0,\ \ s_{in,j_h} \in S_{in,j},\ \ u \in U \tag{3.9}$$

Constraint (3.10) quantifies the heat transferred to the heat storage vessel at the beginning of the time horizon. The initial temperature of the heat storage fluid is $T_0(u, p0)$.

$$Q(s_{in,j_h}, u, p0) = W(u) cp_{fluid} (T_f(u, p1) - T_0(u, p0)) z(s_{in,j_h}, u, p0),$$
$$\forall\, s_{in,j_h} \in S_{in,j}, \quad u \in U \tag{3.10}$$

Constraint (3.11) ensures that the final temperature of the heat storage fluid at any time point becomes the initial temperature of the heat storage fluid at the next time point. This condition will hold regardless of whether or not there was heat integration at the previous time point.

$$T_0(u, p) = T_f(u, p-1), \qquad \forall\, p \in P, \quad u \in U \tag{3.11}$$

Constraints (3.12) and (3.13) ensure that the temperature of heat storage does not change if there is no heat integration with the heat storage unit, unless there is heat loss from the heat storage unit. MM is any large number, thereby resulting in an overall “Big M” formulation. If either $z(s_{in,j_c}, u, p-1)$ or $z(s_{in,j_h}, u, p-1)$ is equal to one, Constraint (3.12) and Constraint (3.13) will be redundant. However, if these two binary variables are both zero, the initial temperature at the previous time point will be equal to the final temperature at the current time point.

$$T_0(u, p-1) \le T_f(u, p) + MM\left(\sum_{s_{in,j_c}} z(s_{in,j_c}, u, p-1) + \sum_{s_{in,j_h}} z(s_{in,j_h}, u, p-1)\right),$$
$$\forall\, p \in P, p > p0, \quad u \in U \tag{3.12}$$

$$T_0(u, p-1) \geq T_f(u, p) - MM\left(\sum_{s_{in,jc}} z(s_{in,j_c}, u, p-1) + \sum_{s_{in,jh}} z(s_{in,j_h}, u, p-1)\right),$$
$$\forall\ p \in P, p > p0, \quad u \in U \tag{3.13}$$

Constraint (3.14) ensures that minimum thermal driving forces are obeyed when there is direct heat integration between a hot and a cold unit. This constraint holds when both hot and cold units operate at constant temperature, which is commonly encountered in practice. An example is when there is heat integration between an exothermic and an endothermic reaction.

$$T(s_{in,j_h}) - T(s_{in,j_c}) \geq \Delta T^{\min} - MM(1 - x(s_{in,j_c}, s_{in,j_h}, p-1)),$$
$$\forall\ p \in P, p > p0, \quad s_{in,j_c}, s_{in,j_h} \in S_{in,j} \tag{3.14}$$

Constraints (3.15) and (3.16) ensure that minimum thermal driving forces are obeyed when there is heat integration with the heat storage unit. Constraint (3.15) applies for heat integration between heat storage and a heat sink, while constraint (3.16) applies for heat integration between heat storage and a heat source. In Constraints (3.15) and (3.16), the units operate at fixed temperatures. For units not operating at fixed temperatures, both inlet and outlet minimal thermal driving forces between the two integrated tasks need also to be enforced.

$$T_f(u, p) - T(s_{in,j_c}) \geq \Delta T^{\min} - MM(1 - z(s_{in,j_c}, u, p-1)),$$
$$\forall\ p \in P, p > p0, \quad s_{in,j_c} \in S_{in,j}, \quad u \in U \tag{3.15}$$

$$T(s_{in,j_h}) - T_f(u, p) \geq \Delta T^{\min} - MM(1 - z(s_{in,j_h}, u, p-1)),$$
$$\forall\ p \in P, p > p0, \ s_{in,j_h} \in S_{in,j}, \quad u \in U \tag{3.16}$$

Constraints (3.17) and (3.18) give the heating load for a cold state and cooling load for a hot state, respectively, for variable batch size and changing temperature.

$$HL(s_{in,j_c}, p) = B(s_{in,j_c}, p)cp_{state}(s_{in,j_c})(T_{out}(s_{in,j_c}) - T_{in}(s_{in,j_c})),$$
$$\forall\ p \in P, \quad s_{in,j_c} \in S_{in,j} \tag{3.17}$$

$$CL(s_{in,j_h}, p) = B(s_{in,j_h}, p)cp_{state}(s_{in,j_h})(T_{in}(s_{in,j_h}) - T_{out}(s_{in,j_h})),$$
$$\forall\ p \in P, \quad s_{in,j_h} \in S_{in,j} \tag{3.18}$$

Constraint (3.19) ensures that the heating of a cold state will be satisfied by either direct or indirect heat integration as well as external utility if required.

$$HL(s_{in,j_c}, p) = Q(s_{in,j_c}, u, p) + st(s_{in,j_c}, p) + \sum_{s_{in,j_h}} q(s_{in,j_c}, s_{in,j_h}, p),$$
$$\forall\ p \in P, \quad s_{in,j_c} \in S_{in,j}, \quad u \in U \tag{3.19}$$

Constraint (3.20) states that the cooling of a hot state will be satisfied by either direct or indirect heat integration as well as external utility if required.

$$CL(s_{in,j_h}, p) = Q(s_{in,j_h}, u, p) + cw(s_{in,j_h}, p) + \sum_{s_{in,j_c}} q(s_{in,j_c}, s_{in,j_h}, p),$$
$$\forall\ p \in P, \quad s_{in,j_h} \in S_{in,j}, \quad u \in U \tag{3.20}$$

The upper bounds of the heating load of a cold state, the cooling load of a hot state and the amount of heat exchanged during direct integration are given in Constraints (3.21) to (3.23).

$$HL(s_{in,j_c}, p) \le y(s_{in,j_c}, p)Q^{\max}(s_{in,j_c}), \qquad \forall\ p \in P, \quad s_{in,j_c} \in S_{in,j} \tag{3.21}$$

$$CL(s_{in,j_h}, p) \le y(s_{in,j_h}, p) Q^{\max}(s_{in,j_h}), \qquad \forall\ p \in P, \quad s_{in,j_h} \in S_{in,j} \tag{3.22}$$

$$q(s_{in,j_c}, s_{in,j_h}, p) \le x(s_{in,j_c}, s_{in,j_h}, p) \min\{Q^{\max}(s_{in,j_c}), Q^{\max}(s_{in,j_h})\}$$
$$\forall\ p \in P, \quad s_{in,j_c}, s_{in,j_h} \in S_{in,j} \tag{3.23}$$

For the specific case where the heating and cooling loads are fixed, Constraints (3.24) and (3.25) are used instead of (3.19) and (3.20).

$$HL(s_{in,j_c}) y(s_{in,j_c}, p) = Q(s_{in,j_c}, u, p) + st(s_{in,j_c}, p)$$
$$+ x(s_{in,j_c}, s_{in,j_h}, p) \sum_{s_{in,j_h}} \min_{s_{in,j_c}, s_{in,j_h}} \{HL(s_{in,j_c}), CL(s_{in,j_h})\},$$
$$\forall\ p \in P, \quad s_{in,j_c} \in S_{in,j}, \quad u \in U \tag{3.24}$$

$$CL(s_{in,j_h}) y(s_{in,j_h}, p) = Q(s_{in,j_h}, u, p) + cw(s_{in,j_h}, p)$$
$$+ x(s_{in,j_c}, s_{in,j_h}, p) \sum_{s_{in,j_c}} \min_{s_{in,j_c}, s_{in,j_h}} \{HL(s_{in,j_c}), CL(s_{in,j_h})\},$$
$$\forall\ p \in P, \quad s_{in,j_h} \in S_{in,j}, \quad u \in U \tag{3.25}$$

The amount of heat transferred through direct heat integration will be limited by the smaller heating or cooling requirement of the heat integrated tasks. Constraints (3.26) and (3.27) express this. Constraint (3.26) calculates the heat load of the cold task, while Constraint (3.27) calculates the cooling load of the hot task.

$$q(s_{in,j_c}, s_{in,j_h}, p) \le B(s_{in,j_c}, p) cp_{state}(s_{in,j_c}) (T_{out}(s_{in,j_c}) - T_{in}(s_{in,j_c})) x(s_{in,j_c}, s_{in,j_h}, p),$$
$$\forall\ p \in P, \quad s_{in,j_c}, s_{in,j_h} \in S_{in,j} \tag{3.26}$$

$$q\left(s_{in,j_c}, s_{in,j_h}, p\right) \leq B\left(s_{in,j_h}, p\right) cp_{state}\left(s_{in,j_h}\right)\left(T_{in}\left(s_{in,j_h}\right) - T_{out}\left(s_{in,j_h}\right)\right) x\left(s_{in,j_c}, s_{in,j_h}, p\right),$$
$$\forall\ p \in P, \quad s_{in,j_c}, s_{in,j_h} \in S_{in,j} \tag{3.27}$$

Furthermore, it is possible that a given pair of tasks cannot be heat integrated or that a possible $\Delta T^{\min}$ violation may occur. In this work, the possibility of heat integration between pairs of tasks as well as possible $\Delta T^{\min}$ violations were investigated for each pair of hot and cold tasks beforehand. If $\Delta T^{\min}$ violations occur, the temperatures in Constraints (3.26) and (3.27) should be adjusted for this.

The amount of heat transferred through direct heat integration can also be limited by the duration of the shorter task if the tasks have different durations. Constraints (3.28) to (3.33) capture this. Constraints (3.28) and (3.29) calculate the heating load per time and cooling load per time, of the cold task and hot task, respectively.

$$\dot{HL}\left(s_{in,j_c}, p\right) = \frac{HL\left(s_{in,j_c}, p\right)}{dur\left(s_{in,j_c}, p\right)}, \qquad \forall\ p \in P, \quad s_{in,j_c} \in S_{in,j} \tag{3.28}$$

$$\dot{CL}\left(s_{in,j_h}, p\right) = \frac{CL\left(s_{in,j_h}, p\right)}{dur\left(s_{in,j_h}, p\right)}, \qquad \forall\ p \in P, \quad s_{in,j_h} \in S_{in,j} \tag{3.29}$$

Constraint (3.30) calculates the heat load of the cold task based on the duration of the same cold task. Constraint (3.31) calculates the heat load of the cold task based on the duration of the hot task. Constraint (3.32) calculates the cooling load of the hot task based on the duration of the same hot task. Constraint (3.33) calculates the cooling load of the hot task based on the duration of the cold task. The amount of heat integrated directly will effectively be the minimum of these four quantities.

$$q\left(s_{in,j_c}, s_{in,j_h}, p\right) \leq \dot{HL}\left(s_{in,j_c}, p\right) dur\left(s_{in,j_c}, p\right), \qquad \forall\ p \in P, \quad s_{in,j_c}, s_{in,j_h} \in S_{in,j} \tag{3.30}$$

$$q\left(s_{in,j_c}, s_{in,j_h}, p\right) \leq \dot{HL}\left(s_{in,j_c}, p\right) dur\left(s_{in,j_h}, p\right), \qquad \forall\ p \in P, \quad s_{in,j_c}, s_{in,j_h} \in S_{in,j} \tag{3.31}$$

$$q\left(s_{in,j_c}, s_{in,j_h}, p\right) \leq \dot{CL}\left(s_{in,j_h}, p\right) dur\left(s_{in,j_h}, p\right), \qquad \forall\ p \in P, \quad s_{in,j_c}, s_{in,j_h} \in S_{in,j} \tag{3.32}$$

$$q\left(s_{in,j_c}, s_{in,j_h}, p\right) \leq \dot{CL}\left(s_{in,j_h}, p\right) dur\left(s_{in,j_c}, p\right), \qquad \forall\ p \in P, \quad s_{in,j_c}, s_{in,j_h} \in S_{in,j} \tag{3.33}$$

In Constraints (3.28) to (3.33), the duration is a function of batch size. If the duration is fixed, $\tau\left(s_{in,j}\right)$ is used and these constraints are then linear.

Constraints (3.34) and (3.35) ensure that the times at which units are active are synchronised when direct heat integration takes place. Starting times for the tasks in the integrated units are the same. This constraint may be relaxed for operations requiring preheating or precooling and is dependent on the process.

$$t_u\left(s_{in,j_h}, p\right) \geq t_u\left(s_{in,j_c}, p\right) - MM\left(1 - x\left(s_{in,j_c}, s_{in,j_h}, p\right)\right)$$
$$\forall\ p \in P, \quad s_{in,j_c}, s_{in,j_h} \in S_{in,j} \tag{3.34}$$

$$t_u\left(s_{in,j_h}, p\right) \leq t_u\left(s_{in,j_c}, p\right) + MM\left(1 - x\left(s_{in,j_c}, s_{in,j_h}, p\right)\right)$$
$$\forall\ p \in P, \quad s_{in,j_c}, s_{in,j_h} \in S_{in,j} \tag{3.35}$$

Constraints (3.36) and (3.37) ensure that if indirect heat integration takes place, the time at which a heat storage unit starts either to transfer or receive heat will be equal to the time a unit is active.

$$t_u\left(s_{in,j}, p\right) \geq t_0\left(s_{in,j}, u, p\right) - MM\left(y\left(s_{in,j}, p\right) - z\left(s_{in,j}, u, p\right)\right)$$
$$\forall\ p \in P, \quad u \in U, \quad s_{in,j} \in S_{in,j} \tag{3.36}$$

$$t_u\left(s_{in,j}, p\right) \le t_0\left(s_{in,j}, u, p\right) + MM\left(y\left(s_{in,j}, p\right) - z\left(s_{in,j}, u, p\right)\right)$$
$$\forall\ p \in P, \quad u \in U, \quad s_{in,j} \in S_{in,j} \tag{3.37}$$

Constraints (3.38) and (3.39) state that the time when heat transfer to or from a heat storage unit is finished will coincide with the time the task transferring or receiving heat has finished processing.

$$t_u\left(s_{in,j}, p-1\right) + \tau\left(s_{in,j}\right) y\left(s_{in,j}, p-1\right) \ge t_f\left(s_{in,j}, u, p\right)$$
$$- MM\left(y\left(s_{in,j}, p-1\right) - z\left(s_{in,j}, u, p-1\right)\right)$$
$$\forall\ p \in P, p > p0, \quad u \in U, \quad s_{in,j} \in S_{in,j} \tag{3.38}$$

$$t_u\left(s_{in,j}, p-1\right) + \tau\left(s_{in,j}\right) y\left(s_{in,j}, p-1\right) \le t_f\left(s_{in,j}, u, p\right)$$
$$+ MM\left(y\left(s_{in,j}, p-1\right) - z\left(s_{in,j}, u, p-1\right)\right)$$
$$\forall\ p \in P, p > p0, \quad u \in U, \quad s_{in,j} \in S_{in,j} \tag{3.39}$$

Wastewater minimisation constraints

The wastewater minimisation constraints are based on the superstructure in Figure 3.1(b). The task being performed in unit $j \in J_w$ is a washing operation in which the water used could consist of freshwater, stored water or recycled/reused water. Water from unit *j* can be recycled into the same unit, reused by other units or sent to storage. Direct water reuse refers to the use of an outlet wastewater stream from one unit in another unit, while indirect water reuse refers to the use of previously stored wastewater in a unit.

Constraints (3.40) to (3.90) constitute the wastewater minimisation model useful for fixed load multipurpose batch processes involving multiple contaminants. The formulation is based on the model by Adekola and Majozi (2011) and includes both direct water reuse and indirect water reuse due to the presence of a central storage vessel.

Mass balances around each processing unit and the central storage vessel are formulated as follows.

Mass balance around a unit

Constraint (3.40) is the water balance over the inlet to a unit. Water entering the unit is a combination of reuse/recycle streams from other units, j', freshwater and water from storage. Constraint (3.41) states that the water leaving a unit could be recycled/reused, sent to storage or discarded as effluent. Constraint (3.42) states that the amount of water exiting a unit must equal the amount of water entering the unit at the previous time point. This constraint captures the fact that water is neither produced nor lost in the unit during the washing operation.

$$mw_{in}(s_{in,j},p) = \sum_{s_{out,j',j}} mw_r(s_{out,j',j},p) + mw_f(s_{in,j},p) + ms_{out}(j,p)$$
$$\forall\ j,j' \in J_w,\ s_{in,j} \in S_{in,j},\ \ p \in P \qquad (3.40)$$

$$mw_{out}(s_{out,j},p) = \sum_{s_{out,j,j'}} mw_r(s_{out,j,j'},p) + mw_e(s_{out,j},p) + ms_{in}(j,p)$$
$$\forall\ j,j' \in J_w,\ \ s_{out,j} \in S_{out,j},\ p \in P \qquad (3.41)$$

$$mw_{in}(s_{in,j},p-1) = mw_{out}(s_{out,j},p)$$
$$\forall\ j \in J_w,\ s_{in,j} \in S_{in,j},\ s_{out,j} \in S_{out,j},\ p \in P,\ p > p0 \qquad (3.42)$$

Constraint (3.43) represents the inlet contaminant mass balance. The contaminant mass load in the inlet stream is the sum of the contaminant mass load in recycle/reuse water and that in water from storage. Constraint (3.44) represents the outlet contaminant mass as the sum of the mass of contaminant that entered the unit at the previous time point and the mass load of contaminant picked up in the unit during washing. In Constraint (3.44), the mass load of contaminant in a unit is a given parameter.

$$mw_{in}(s_{in,j}, p)c_{in}(s_{in,j}, c, p) = \sum_{s_{out,j',j}} mw_r(s_{out,j',j}, p)c_{out}(s_{out,j'}, c, p)$$
$$+ms_{out}(j, p)cs_{out}(c, p)$$
$$\forall\ j, j' \in J_w,\ s_{in,j} \in S_{in,j},\ s_{out,j',j} \in S_{out,j',j},\ p \in P, c \in C \qquad (3.43)$$

$$mw_{out}(s_{out,j}, p)c_{out}(s_{out,j}, c, p) = M(s_{in,j}, c)yw(s_{out,j}, p-1)$$
$$+ mw_{in}(s_{in,j}, p-1)c_{in}(s_{in,j}, c, p-1)$$
$$\forall\ j \in J_w,\ s_{in,j} \in S_{in,j},\ s_{out,j} \in S_{out,j},\ p \in P,\ p > p_1, c \in C \qquad (3.44)$$

In the case where the mass load of contaminant in a unit is defined as a function of batch size of material processed in the unit, Constraint (3.45) represents the outlet contaminant mass. Constraint (3.46) defines the variable contaminant mass load as the product of the contaminant loading and the batch size of material processed.

$$mw_{out}(s_{out,j}, p)c_{out}(s_{out,j}, c, p) = M_B(s_{in,j}, c, p-1)yw(s_{in,j}, p-1)$$
$$+ mw_{in}(s_{in,j}, p-1)c_{in}(s_{in,j}, c, p-1)$$
$$\forall\ j \in J_w,\ s_{in,j} \in S_{in,j},\ s_{out,j} \in S_{out,j},\ p \in P,\ p > p_1, c \in C \qquad (3.45)$$

$$M_B(s_{in,j}, c, p) = A(c)B(s_{in,j}, p)$$
$$\forall\ j \in J_w,\ s_{in,j} \in S_{in,j},\ p \in P,\ c \in C \qquad (3.46)$$

Constraints (3.47) and (3.48) ensure that the inlet and outlet contaminant concentrations do not exceed the allowed maximum. Similarly, the maximum allowable water in a unit must not be exceeded. This is governed by Constraint (3.49). Constraint (3.50) restricts the mass of water entering the unit from recycle/reuse to the maximum allowable for the unit. Likewise, Constraint (3.51) restricts the mass of water entering the unit from storage to the maximum allowable for the unit.

$$c_{in}\left(s_{in,j},c,p\right)\leq C_{in}^{U}\left(s_{in,j},c\right)yw\left(s_{in,j},p\right)$$
$$\forall\ j\in J_{w},s_{in,j}\in S_{in,j},p\in P,c\in C \tag{3.47}$$

$$c_{out}\left(s_{out,j},c,p\right)\leq C_{out}^{U}\left(s_{out,j},c\right)yw\left(s_{in,j},p-1\right)$$
$$\forall\ j\in J_{w},s_{in,j}\in S_{in,j},s_{out,j}\in S_{out,j},p\in P,p>p_{1},c\in C \tag{3.48}$$

$$mw_{in}\left(s_{in,j},p\right)\leq Mw^{U}\left(s_{in,j}\right)yw\left(s_{in,j},p\right)\qquad \forall\ j\in J_{w},s_{in,j}\in S_{in,j},p\in P \tag{3.49}$$

$$mw_{r}\left(s_{out,j',j},p\right)\leq Mw^{U}\left(s_{in,j}\right)yw_{r}\left(s_{out,j',j},p\right)$$
$$\forall\ j,j'\in J_{w},s_{in,j}\in S_{in,j},s_{out,j',j}\in S_{out,j',j},p\in P \tag{3.50}$$

$$ms_{out}\left(s_{out,j},p\right)\leq Mw^{U}\left(s_{in,j}\right)ys_{out}\left(s_{out,j},p\right)$$
$$\forall\ j\in J_{w},s_{in,j}\in S_{in,j},s_{out,j}\in S_{out,j},p\in P \tag{3.51}$$

The maximum quantity of water into a unit is calculated using Equation (3.52). It is important to note that for multicontaminant wastewater the outlet concentration of the individual components cannot all be set to the maximum, since the contaminants are not limiting simultaneously. The limiting contaminant(s) will always be at the maximum outlet concentration and the non-limiting contaminants will be below their respective maximum outlet concentrations.

$$Mw^{U}\left(s_{in,j}\right)=\max_{c\in C}\left\{\frac{M\left(s_{in,j},c\right)}{C_{out}^{U}\left(s_{out,j},c\right)-C_{in}^{U}\left(s_{in,j},c\right)}\right\}$$
$$\forall\ j\in J_{w},s_{in,j}\in S_{in,j},s_{out,j}\in S_{out,j},c\in C \qquad (3.52)$$

Mass balance around central storage

Constraint (3.53) is the water mass balance around the storage tank. The amount of water stored in the storage tank consists of water stored at the previous time point and the difference between water entering the storage tank from a unit and water leaving the storage tank to a unit. Constraint (3.54) defines the initial amount of water in the tank.

$$qw_{s}(p)=qw_{s}(p-1)+\sum_{j\in J_{w}}ms_{in}(j,p)-\sum_{j\in J_{w}}ms_{out}(j,p)\quad \forall\ p\in P,\ p>p0 \qquad (3.53)$$

$$qw_{s}(p0)=Qw_{s}^{o}-\sum_{j\in J_{w}}ms_{out}(j,p0) \qquad (3.54)$$

The definition of the inlet contaminant concentration to the storage tank is given in Constraint (3.55). The concentration of water exiting the storage tank is assumed to be equal to the concentration of water in the tank as given in Constraint (3.56). This condition is true in the case of perfect mixing. The initial concentration in the storage tank is expressed in Constraint (3.57). Constraint (3.58) ensures that the maximum capacity of the tank is not exceeded.

$$cs_{in}(c,p)=\frac{\sum_{j\in J_{w}}\left(ms_{in}(j,p)c_{out}\left(s_{in,j},c,p\right)\right)}{\sum_{j\in J_{w}}ms_{in}(j,p)}$$
$$\forall\ s_{in,j}\in S_{in,j},p\in P,c\in C \qquad (3.55)$$

$$cs_{out}(c,p)=\frac{qw_s(p-1)cs_{out}(c,p-1)+\left[\sum_{j\in J_w} ms_{in}(j,p)\right]cs_{in}(c,p)}{qw_s(p-1)+\sum_{j\in J_w} ms_{in}(j,p)}$$

$$\forall\ p\in P,\ p\geq p0,\ c\in C \tag{3.56}$$

$$cs_{out}(c,p0)=CS_{out}^{o}(c) \qquad \forall c\in C \tag{3.57}$$

$$qw_s(p)\leq Qw_s^U \qquad \forall\ p\in P \tag{3.58}$$

Constraint (3.59) ensures that no water is stored in the storage vessel at the end of the time horizon in order to give a true optimum. Otherwise the resulting minimum effluent could be misleading.

$$qw_s(p)=0 \quad \forall\ p=|P| \tag{3.59}$$

The scheduling constraints for the wastewater minimisation model are as follows.

Task scheduling constraints

Unlike heating or cooling that can occur during a production task, a unit can only perform either a production task or a washing task at any given point in time. The task scheduling constraints ensure the proper sequencing of equipment washing and production tasks. Constraint (3.60) expresses the duration of the production task (Majozi & Zhu, 2001). Constraint (3.61) stipulates that washing can only commence at time point p if the unit was active at the previous time point performing a production task, i.e. $y(s_{in,j},p-1)$ has a value of 1. Constraints (3.62) and (3.63) together ensure that unit j is washed immediately after a production task, which produced $s_{out,j}$, has ended in the unit. If washing is being performed in the unit, $yw(s_{in,j}, p)$ has a value of 1 causing Constraints (3.62) and (3.63) to become active and the start time of washing is forced to coincide with the end time of production. Otherwise, when water is not used in the unit, i.e. $yw(s_{in,j}, p)$ has a value of zero, the two constraints become relaxed. Constraint (3.64) represents the duration of the washing task performed in unit *j*.

$$t_{out}(s_{out,j}, p) = t_u(s_{in,j}, p-1) + \tau(s_{in,j})y(s_{in,j}, p-1)$$
$$\forall\ j \in J_w,\ s_{in,j} \in S_{in,j},\ s_{out,j} \in S_{out,j},\ p \in P,\ p > p0 \qquad (3.60)$$

$$yw(s_{in,j}, p) = y(s_{in,j}, p-1) \qquad \forall\ j \in J_w,\ s_{in,j} \in S_{in,j},\ p \in P,\ p > p0 \qquad (3.61)$$

$$tw_{in}(s_{in,j}, p) \geq t_{out}(s_{out,j}, p) - MM(1 - yw(s_{in,j}, p))$$
$$\forall\ j \in J_w,\ s_{in,j} \in S_{in,j},\ s_{out,j} \in S_{out,j},\ p \in P \qquad (3.62)$$

$$tw_{in}(s_{in,j}, p) \leq t_{out}(s_{out,j}, p) + MM(1 - yw(s_{in,j}, p))$$
$$\forall\ j \in J_w,\ s_{in,j} \in S_{in,j},\ s_{out,j} \in S_{out,j},\ p \in P \qquad (3.63)$$

$$tw_{out}(s_{out,j}, p) = tw_{in}(s_{in,j}, p-1) + \tau w(s_{in,j})yw(s_{in,j}, p-1)$$
$$\forall\ j \in J_w,\ s_{in,j} \in S_{in,j},\ s_{out,j} \in S_{out,j},\ p \in P,\ p > p0 \qquad (3.64)$$

Recycle/reuse scheduling

Wastewater can only be recycled/reused directly if the unit producing wastewater and the unit receiving wastewater finish operating and begin operating at the same time, respectively. Constraint (3.65) describes the relationship between usage of water in a unit and the opportunity for recycle and reuse. The constraint states that for a unit *j* to transfer water to unit j', unit j' should require water at that time point. It does not, however, mean that unit j' must use water from unit j, it could still obtain water from other sources. Constraints (3.66) and (3.67) state that the time at which water recycle/ reuse takes place coincides with the time at which the water is produced. Constraints (3.68) and (3.69) ensure that the time at which water recycle/reuse takes place coincides with the starting time of the unit receiving the water.

$$yw_r(s_{out,j,j'}, p) \le yw(s_{in,j'}, p)$$
$$\forall\ j, j' \in J_w,\ s_{in,j} \in S_{in,j},\ s_{out,j,j'} \in S_{out,j,j'},\ p \in P \tag{3.65}$$

$$tw_r(s_{out,j,j'}, p) \le tw_{out}(s_{out,j}, p) - MM(1 - yw_r(s_{out,j,j'}, p))$$
$$\forall\ j, j' \in J_w,\ s_{out,j} \in S_{out,j},\ s_{out,j,j'} \in S_{out,j,j'},\ p \in P \tag{3.66}$$

$$tw_r(s_{out,j,j'}, p) \ge tw_{out}(s_{out,j}, p) + MM(1 - yw_r(s_{out,j,j'}, p))$$
$$\forall\ j, j' \in J_w,\ s_{out,j} \in S_{out,j},\ s_{out,j,j'} \in S_{out,j,j'},\ p \in P \tag{3.67}$$

$$tw_r(s_{out,j,j'}, p) \le tw_{in}(s_{in,j'}, p) - MM(1 - yw_r(s_{out,j,j'}, p))$$
$$\forall\ j, j' \in J_w, s_{in,j} \in S_{in,j}, s_{out,j,j'} \in S_{out,j,j'}, p \in P \tag{3.68}$$

$$tw_r(s_{out,j,j'}, p) \ge tw_{in}(s_{in,j'}, p) + MM(1 - yw_r(s_{out,j,j'}, p))$$
$$\forall\ j, j' \in J_w, s_{in,j} \in S_{in,j}, s_{out,j,j'} \in S_{out,j,j'}, p \in P \tag{3.69}$$

Central storage scheduling

Constraint (3.70) relates water usage in a unit and water transfer from storage. It states that water can only be transferred to a unit if it uses water at the same time point. However, it is not a prerequisite for the unit to use stored water, the water could be provided from other sources. Constraints (3.71) and (3.72) ensure that the time at which water is sent from storage to a unit coincides with the start time of washing of the unit.

$$ys_{out}(j,p) \leq yw(s_{in,j},p) \qquad \forall\ j \in J_w,\ s_{in,j} \in S_{in,j},\ p \in P \tag{3.70}$$

$$ts_{out}(j,p) \geq tw_{in}(s_{in,j},p) - MM(2 - ys_{out}(j,p) - yw(s_{in,j},p))$$
$$\forall\ j \in J_w, s_{in,j} \in S_{in,j}, p \in P \tag{3.71}$$

$$ts_{out}(j,p) \leq tw_{in}(s_{in,j},p) + MM(2 - ys_{out}(j,p) - yw(s_{in,j},p))$$
$$\forall\ j \in J_w,\ s_{in,j} \in S_{in,j},\ p \in P \tag{3.72}$$

Constraint (3.73) relates water usage in a unit and water transfer to storage. It states that water can only be transferred from a unit to storage if the unit used water at the previous time point. However, washing can take place in the unit without discharging water to the storage tank. The water could be discharged to other sinks. Constraints (3.74) and (3.75) ensure that the time at which water is sent to storage from a unit must coincide with the finishing time of washing of the unit.

$$ys_{in}(j,p) \leq yw(s_{in,j},p-1) \qquad \forall\ j \in J_w,\ s_{in,j} \in S_{in,j},\ p \in P,\ p > p_1 \tag{3.73}$$

$$ts_{in}(j,p) \geq tw_{out}(s_{out,j},p) - MM(2 - ys_{in}(j,p) - yw(s_{in,j},p-1))$$
$$\forall\ j \in J_w,\ s_{in,j} \in S_{in,j},\ s_{out,j} \in S_{out,j},\ p \in P,\ p > p_1 \tag{3.74}$$

$$ts_{in}(j,p) \leq tw_{out}(s_{out,j},p) + MM(2 - ys_{in}(j,p) - yw(s_{in,j},p-1))$$
$$\forall\ j \in J_w,\ s_{in,j} \in S_{in,j},\ s_{out,j} \in S_{out,j},\ p \in P,\ p > p_1 \tag{3.75}$$

If water is transferred from storage to a unit at a later time point, the time at which this happens must correspond to a later time in the time horizon. This is specified in Constraint (3.76). Constraint (3.77) ensures that if water is transferred from a unit to storage at a later time point, the time at which this happens corresponds to a later time in the time horizon.

$$ts_{out}(j,p) \geq ts_{out}(j',p') - MM(2 - ys_{out}(j,p) - ys_{out}(j',p'))$$
$$\forall\ j,j' \in J_w,\ p,p' \in P,\ p \geq p' \tag{3.76}$$

$$ts_{in}(j,p) \geq ts_{in}(j',p') - MM(2 - ys_{in}(j,p) - ys_{in}(j',p'))$$
$$\forall\ j,j' \in J_w,\ p,p' \in P,\ p \geq p' \tag{3.77}$$

Constraints (3.78) and (3.79) state that if water is transferred to storage from more than one unit at the same time point, the time at which they do so must coincide. Constraints (3.80) and (3.81) state that if water is discharged from storage to more than one unit at the same time point, the time at which the water is discharged must coincide.

$$ts_{in}(j,p) \geq ts_{in}(j',p) - MM(2 - ys_{in}(j,p) - ys_{in}(j',p))$$
$$\forall\ j,j' \in J_w,\ p \in P \tag{3.78}$$

$$ts_{in}(j,p) \leq ts_{in}(j',p) + MM(2 - ys_{in}(j,p) - ys_{in}(j',p))$$
$$\forall\ j,j' \in J_w,\ p \in P \tag{3.79}$$

$$ts_{out}(j,p) \geq ts_{out}(j',p) - MM(2 - ys_{out}(j,p) - ys_{out}(j',p))$$
$$\forall\ j,j' \in J_w,\ p \in P \tag{3.80}$$

$$ts_{out}(j,p) \le ts_{out}(j',p) + MM(2 - ys_{out}(j,p) - ys_{out}(j',p))$$
$$\forall\ j, j' \in J_w,\ p \in P \tag{3.81}$$

If water is simultaneously being transferred to and discharged from storage, the time at which this happens should coincide. This is given in Constraints (3.82) and (3.83).

$$ts_{in}(j,p) \ge ts_{out}(j',p) - MM(2 - ys_{in}(j,p) - ys_{out}(j',p))$$
$$\forall\ j, j' \in J_w,\ p \in P \tag{3.82}$$

$$ts_{in}(j,p) \le ts_{out}(j',p) + MM(2 - ys_{in}(j,p) - ys_{out}(j',p))$$
$$\forall\ j, j' \in J_w,\ p \in P \tag{3.83}$$

Constraint (3.84) ensures that if water leaves storage at a later time point compared to water entering the storage, the time at which water leaves the storage must correspond to a later time in the time horizon.

$$ts_{out}(j,p) \ge ts_{in}(j',p') - MM(2 - ys_{out}(j,p) - ys_{in}(j',p'))$$
$$\forall\ j, j' \in J_w,\ p, p' \in P,\ p \ge p' \tag{3.84}$$

The following feasibility and time horizon constraints also hold. Constraint (3.85) ensures that if a processing unit j is reusing water from unit j' at time point p, then unit j' cannot reuse water from unit j at the same time point.

$$yw_r(s_{out,j,j'}, p) + yw_r(s_{out,j',j}, p) \le 1$$
$$\forall\ j, j' \in J_w,\ s_{out,j,j'}, s_{out,j',j} \in S_{out,j,j'},\ p \in P \tag{3.85}$$

Constraints (3.86) to (3.90) ensure that each event occurs within the time horizon of interest.

$$tw_{in}\left(s_{in,j}, p\right) \le H \qquad \forall\ j \in J_w,\ s_{in,j} \in S_{in,j},\ p \in P \tag{3.86}$$

$$tw_{out}\left(s_{out,j}, p\right) \le H \qquad \forall\ j \in J_w,\ s_{out,j} \in S_{out,j},\ p \in P \tag{3.87}$$

$$tw_{r}\left(s_{out,j,j'}, p\right) \le H \qquad \forall\ j \in J_w,\ s_{out,j,j'} \in S_{out,j,j'},\ p \in P \tag{3.88}$$

$$ts_{in}\left(s_{in,j}, p\right) \le H \qquad \forall\ j \in J_w,\ s_{in,j} \in S_{in,j},\ p \in P \tag{3.89}$$

$$ts_{out}\left(s_{out,j}, p\right) \le H \qquad \forall\ j \in J_w,\ s_{out,j} \in S_{out,j},\ p \in P \tag{3.90}$$

The objective of the formulation is either the maximisation of profit or the minimisation of makespan. Constraint (3.91) expresses the profit as the difference between the product revenue and the sum of freshwater, effluent treatment, cooling water and steam costs. When the objective is the maximisation of profit, Constraint (3.91) is maximised. As a result, the sum of external utilities and freshwater consumption is minimised.

$$\begin{aligned}\text{Profit} = &\sum_{s}\sum_{p} CP(s)d(s,p) - CF\sum_{s_{in,j}}\sum_{p} mw_f\left(s_{in,j}, p\right) - CE\sum_{s_{out,j}}\sum_{p} mw_e\left(s_{out,j}, p\right) \\ &- Cost\_cw\sum_{s_{in,jh}}\sum_{p} cw\left(s_{in,jh}, p\right) - Cost\_st\sum_{s_{in,jc}}\sum_{p} st\left(s_{in,jc}, p\right)\end{aligned} \tag{3.91}$$

Constraint (3.92) is the objective function for makespan minimisation. In Constraint (3.92), the quotient of profit and time horizon is maximised. As a result, the makespan is minimised and the sum of the external utilities used and freshwater consumed is minimised using the same reasoning as above. The numerator (profit) will tend to increase, while the denominator (makespan) will tend to decrease.

$$Max\ \frac{Profit}{H} \tag{3.92}$$

3.4 Solution procedure

The overall model, whether for a profit maximisation problem or a makespan minimisation problem is a MINLP. When solving a profit maximisation problem, the model is linearised and solved as a MILP, the solution of which is then used as a starting point for the exact MINLP model. If the solutions from the two models are equal, the solution is globally optimal, as global optimality can be proven for MILP problems. If the solutions differ, the MINLP solution is locally optimal. The possibility also exists that no feasible starting point is found. This solution procedure was used by Gouws *et al.* (2008), Adekola and Majozi (2011) and Stamp and Majozi (2011) and is shown graphically in Figure 3.2.

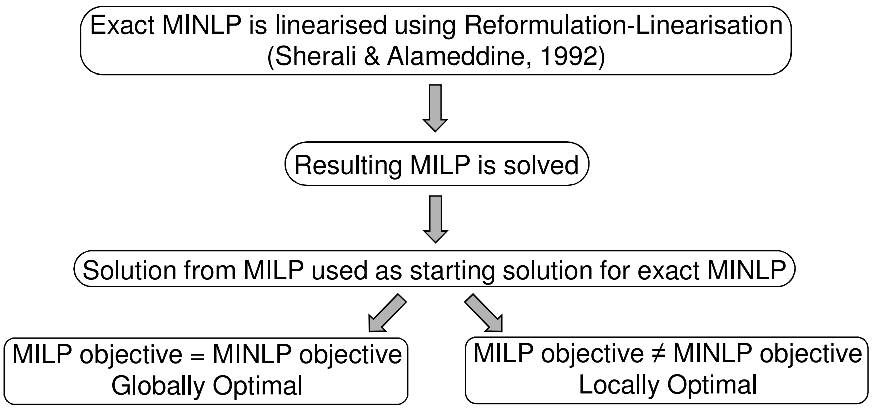

Figure 3.2. Solution algorithm for Reformulation-Linearisation technique.

When solving a makespan minimisation problem, the MINLP cannot be linearised completely to a MILP due to the nonlinear objective function, Constraint (3.92). The MINLP is therefore linearised to a relaxed MINLP problem which provides a starting point for the exact MINLP problem. However, the resulting solution to the exact MINLP cannot be guaranteed to be a global optimum.

Constraints (3.8), (3.9) and (3.10) have trilinear terms where a binary variable and two continuous variables are multiplied. Constraints (3.28) to (3.33), (3.43) to (3.45), (3.55) and

(3.56) have bilinear terms where two continuous variables are multiplied. This results in a nonconvex MINLP formulation. The bilinearity resulting from the multiplication of a continuous variable with a binary variable as found in Constraints (3.26) and (3.27) may be handled effectively with the Glover transformation (Glover, 1975). This is an exact linearisation technique and as such will not compromise the accuracy of the model. The procedure is demonstrated for Constraint (3.9).

Let

$$T_f(u,p)z(s_{in,j_h},u,p-1)=\Gamma_1(s_{in,j_h},u,p) \tag{3.93}$$

With lower and upper temperature bounds known

$$T^L \leq T_f(u,p) \leq T^U \tag{3.94}$$

Then

$$\Gamma_1(s_{in,j_h},u,p) \geq T_f(u,p) - T^U\left(1 - z(s_{in,j_h},u,p-1)\right) \tag{3.95}$$

$$\Gamma_1(s_{in,j_h},u,p) \leq T_f(u,p) + T^L\left(1 - z(s_{in,j_h},u,p-1)\right) \tag{3.96}$$

$$\Gamma_1(s_{in,j_h},u,p) \geq z(s_{in,j_h},u,p-1)T^L \tag{3.97}$$

$$\Gamma_1(s_{in,j_h},u,p) \leq z(s_{in,j_h},u,p-1)T^U \tag{3.98}$$

The result from the Glover transformation for Constraint (3.9) is seen in Constraint (3.99) and includes the addition of one new continuous variable and four new continuous constraints.

$$Q\left(s_{in,j_h}, u, p-1\right) = W(u) cp_{fluid}\left(\Gamma_1\left(s_{in,j_h}, u, p\right) - \Gamma_2\left(s_{in,j_h}, u, p-1\right)\right),$$
$$\forall\ p \in P, p > p0,\quad s_{in,j_h} \in S_{in,j},\quad u \in U \tag{3.99}$$

The heat storage capacity, $W(u)$, is also a continuous variable and is multiplied with the continuous Glover transformation variable. This results in another type of bilinearity, which results in a nonconvex model. A method to handle this is a Reformulation-Linearisation technique (Sherali & Alameddine, 1992) as discussed by Quesada and Grossmann (1995). This is demonstrated for Constraint (3.99), resulting in Constraints (3.100) to (3.107).

Let

$$W(u)\Gamma_1\left(s_{in,j_h}, u, p\right) = \Psi_1\left(s_{in,j_h}, u, p\right) \tag{3.100}$$

With lower and upper heat storage capacity and temperature bounds known

$$W^L \leq W(u) \leq W^U \tag{3.101}$$

$$T^L \leq \Gamma_1\left(s_{in,j_h}, u, p\right) \leq T^U \tag{3.102}$$

Then

$$\Psi_1\left(s_{in,j_h}, u, p\right) \geq W^L \Gamma_1\left(s_{in,j_h}, u, p\right) + T^L W(u) - W^L T^L \tag{3.103}$$

$$\Psi_1\left(s_{in,j_h}, u, p\right) \geq W^U \Gamma_1\left(s_{in,j_h}, u, p\right) + T^U W(u) - W^U T^U \tag{3.104}$$

$$\Psi_1\left(s_{in,j_h}, u, p\right) \leq W^U \Gamma_1\left(s_{in,j_h}, u, p\right) + T^L W(u) - W^U T^L \tag{3.105}$$

$$\Psi_1\left(s_{in,j_h},u,p\right) \leq W^L \Gamma_1\left(s_{in,j_h},u,p\right) + T^U W(u) - W^L T^U \tag{3.106}$$

This is an inexact linearisation technique and increases the size of the model by an additional type of continuous variable and four types of continuous constraints. These constraints correspond to the convex and concave envelopes of the bilinear terms over the given bounds.

The final completely linearised form of Constraint (3.9) can be seen in Constraint (3.107).

$$Q\left(s_{in,j_h},u,p-1\right) = cp_{fluid}\left(\Psi_1\left(s_{in,j_h},u,p\right) - \Psi_2\left(s_{in,j_h},u,p-1\right)\right)$$
$$\forall\ p \in P, p > p0,\quad s_{in,j_h} \in S_{in,j},\quad u \in U \tag{3.107}$$

Bounds on the heat storage capacity will be determined by the available space in the plant, as batch plants usually operate in limited space.

For the profit maximisation problem, the linearisation procedure is carried out for each of the nonlinear terms in Constraints (3.8) to (3.10), (3.26) to (3.33), (3.43) to (3.45), (3.55) and (3.56) to produce a MILP problem, which provides a starting point for the exact MINLP problem. The objective function for the makespan minimisation problem is also nonlinear, however, and only Constraints (3.8) to (3.10), (3.26) to (3.33), (3.43) to (3.45), (3.55) and (3.56) are linearised to produce a relaxed MINLP problem, the solution of which provides a starting point for the exact MINLP problem.

3.5 Case study I (Halim & Srinivasan, 2011)

This case study is a simple sequential process. A single product is produced via three tasks in five units. The case study has been adapted to include water and energy using operations. Figure 3.3 shows the recipe representation of the process. Steam is available for heating, cooling water is available for cooling and freshwater is available for washing. The objective is to maximise profit over a 12 h time horizon, while minimising the sum of the utility requirements and freshwater usage.

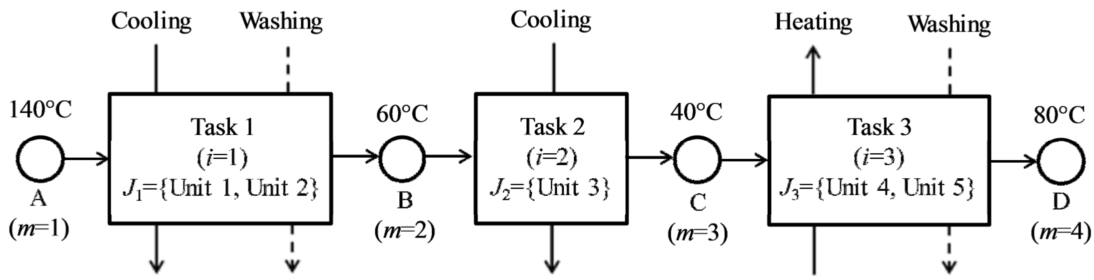

Figure 3.3. Recipe representation of the simple sequential process for case study I.

Data required for case study I may be obtained from Table 3.1 to Table 3.3.

Table 3.1. Data pertaining to production, for case study I.

Task (i)	Unit (j)	Max batch size (kg)	Processing time (h)	Washing time (h)	Material state (m)	Initial inventory (kg)	Max storage (kg)	Revenue/ cost ($/kg or $/MJ)
Task 1	Unit 1	100	1.25	0.25	A	1000	1000	0
	Unit 2	150	1.70	0.30	B	0	200	0
Task 2	Unit 3	200	1.50	0	C	0	250	0
Task 3	Unit 4	100	0.75	0.25	D	0	1000	5
	Unit 5	150	1.20	0.30	Washwater			0.1
					Wastewater			0.05
					Cooling water			0.02
					Steam			1

Table 3.2. Data pertaining to energy requirements, for case study I.

Task (i)	T_{in} (°C)	T_{out} (°C)	Unit (j)	cp (kJ/kg°C)
Task 1	140	60	Unit 1	4.0
			Unit 2	4.0
Task 2	60	40	Unit 3	3.5
Task 3	40	80	Unit 4	3.0
			Unit 5	3.0
Cooling water	20	30		
Steam	170	160		

Table 3.3. Data pertaining to water requirements, for case study I.

Task (*i*)	Unit (*j*)	Max inlet concentration (ppm)	Max outlet concentration (ppm)	Contaminant loading (g contaminant/kg batch)
Task 1	Unit 1	500	1000	0.2
	Unit 2	50	100	0.2
Task 2	Unit 3	-	-	0.2
Task 3	Unit 4	150	300	0.2
	Unit 5	300	2000	0.2

The following should be noted:

1. The processing duration of a batch is fixed.
2. The mass load of contaminants is dependent on the batch size.
3. A single contaminant is present.
4. The energy requirements of the operations are a function of the batch size and the given initial and final temperatures. Due to this fact, careful consideration must be given to ensure that whenever heat integration occurs between two operations, the minimum temperature difference for heat transfer, 10°C, is not violated.

The first case study was solved with the proposed formulation, using Constraints (3.1), (3.2), (3.17) to (3.23), (3.26) to (3.35), (3.40) to (3.43) and (3.45) to (3.50), (3.52), (3.60) to (3.69) and (3.85) to (3.88). The objective function was the maximisation of Constraint (3.91). It is important to note that in Constraints (3.40), (3.41), (3.43) and (3.45), variables associated with wastewater storage are not included. Due to the fact that a single contaminant was present, the formulation for this case study could be reduced to a MILP. The outlet contaminant concentration was fixed to the maximum, Constraint (3.43) was substituted into Constraint (3.45) and a Glover transformation was performed on the resulting equation (Majozi, 2005). The computer used to solve the model had an Intel(R) Core(TM) i7-2670QM, 2.2 GHz processor with 4.0 GB RAM. The problem was solved with GAMS using CPLEX as the MIP solver.

The results from the first case study as compared to the results achieved by Halim and Srinivasan (2011) may be obtained from Table 3.4.

Table 3.4. Comparison of results for case study I.

	Halim & Srinivasan (2011)	This formulation
Profit ($)	4 764.1	4 775.28
Steam (MJ)	43.9	66
Cooling water (MJ)	313.9	336
Total freshwater (kg)	1 238.37	1 013.33
Revenue from product ($)	5 000	5 000
Cost of steam ($)	43.9	66
Cost of cooling water ($)	6.28	6.72
Cost of freshwater ($)	123.8	101.3
Cost of wastewater ($)	61.9	50.7
Number of slots	7	N/A
Number of time points	N/A	15
Number of binary variables	not reported	385
Number of iterations	1 500	N/A
CPU time (s)	not reported	28 797

As can be observed from Table 3.4, a better profit overall was obtained with the proposed formulation. Although the amounts for steam and cooling water were lower for the model by Halim and Srinivasan (2011), the amount of freshwater required was lower in the proposed formulation, which also results in a lower effluent production. This is a consequence of differences in the schedule obtained by Halim and Srinivasan (2011) compared to the current formulation. The advantage of the current work is that the variable nature of time ensures that the schedule is flexible and results that could have been overlooked when time is fixed are available during the optimisation search. The CPU time required to solve the problem was approximately 8 h. This highlights the complexity introduced by solving scheduling, wastewater minimisation and heat integration simultaneously, whereas the standalone scheduling problem resulted in an objective of $5000 obtained in 0.097 s.

Similar to the method by Halim and Srinivasan (2011), the washing of a unit may not necessarily occur immediately after the end of a processing task, but can be delayed to improve reuse opportunities with other units. To cater for this, Constraint (3.63) was removed from the formulation while Constraint (3.62) remained.

Figure 3.4 shows the Gantt chart with the resulting production schedule for the first case study. The clear horizontal blocks represent the tasks associated with production processes. The amount of material processed in each unit is labelled above the clear blocks. The dark horizontal blocks represent the washing of a unit. The amount of water associated with washing is labelled underneath the relevant dark blocks. The double sided arrows (up-down arrows) represent direct heat integration between two tasks. The numbers in round brackets represent the amount of energy associated with heat integration. The numbers in curly brackets represent steam duties while the numbers in square brackets represent cooling water duties.

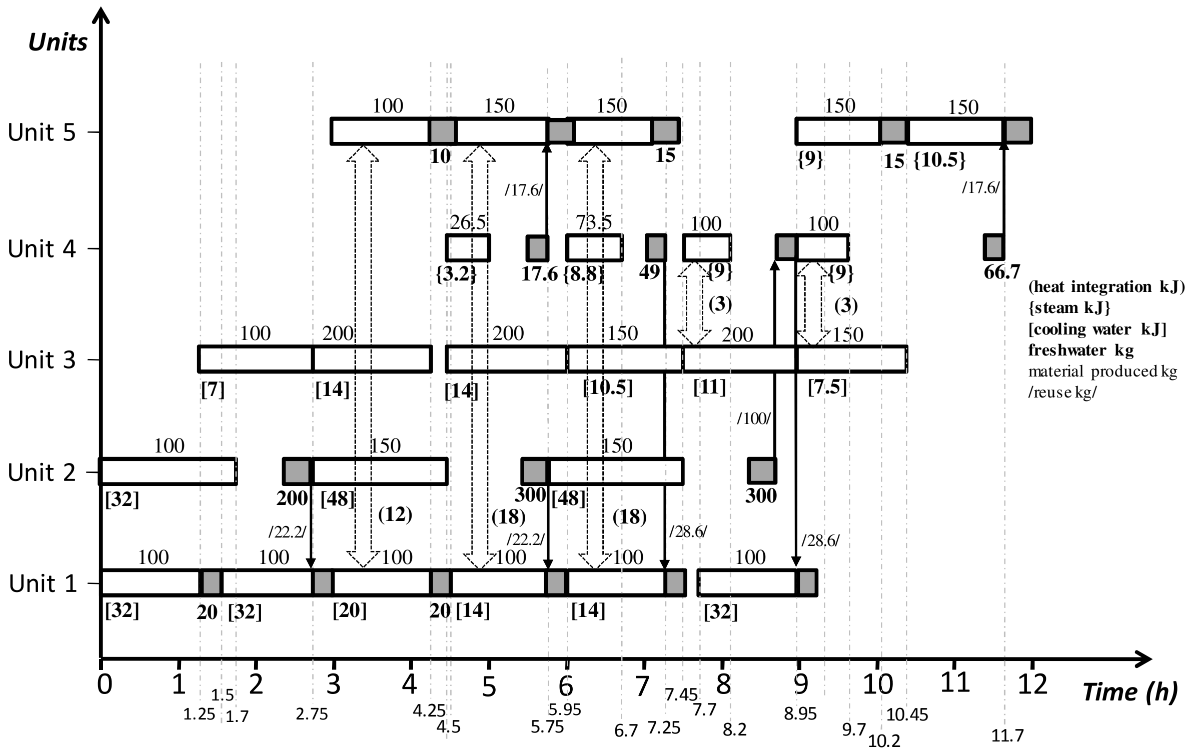

Figure 3.4. Resulting production schedule for case study I.

3.6 Case study II

This case study comprises of the popular literature example by Kondili *et al.* (1993). Halim and Srinivasan (2011) adapted this complex production process to include energy and water using aspects and it is described here. For the production process, two products, Product 1 and Product 2 are to be produced from three raw materials: Feed A, Feed B and Feed C. A heater, HR is used to heat Feed A. Two reactors, RR1 and RR2 are available to perform three different chemical reactions, Reaction 1, Reaction 2 and Reaction 3. Finally, a separator exists to purify Impure E. Figure 3.5 shows the STN representation of the problem. Steam is available for heating, cooling water is available for cooling and freshwater is available for washing. The production recipe is as follows:

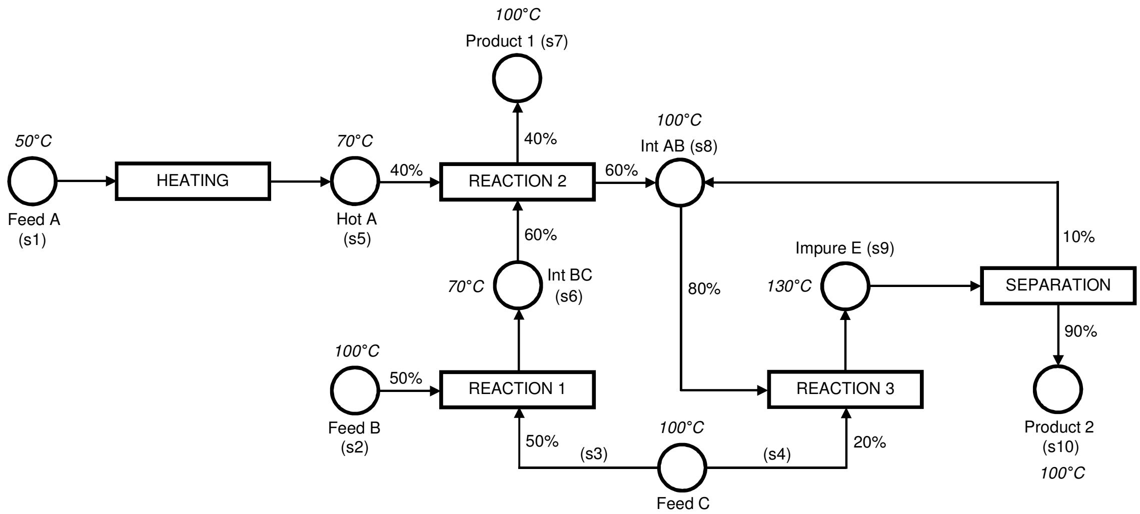

Figure 3.5. STN representation of the complex production facility for case study II.

1. Heating: Feed A is heated from 50°C to 70°C inside HR. Steam is required as a heating medium for this reaction.

2. Reaction 1: A mixture of 50% Feed B and 50% Feed C, on a mass basis, is reacted in either unit RR1 or RR2. The product of this reaction is Int BC. The reaction requires cooling from 100°C to 70°C.

3. Reaction 2: A mixture of 40% Hot A and 60% Int BC is reacted to form Prod 1 (40%) and Int AB (60%). This reaction can be performed in either unit RR1 or RR2 and requires heating from 70°C to 100°C.
4. Reaction 3: A mixture of 20% Feed C and 80% Int AB is reacted in either unit RR1 or RR2. The reaction produces Impure E and requires heating from 100°C to 130°C.
5. Separation: In SR, Impure E is purified to produce Prod 2 (90%) and intermediate Int AB (10%). The separation requires cooling from 130°C to 100°C.

Water is required for washing RR1 and RR2 at the end of any reaction. In this case study, four contaminants, ar, br, cp and dw are present. Table 3.5 shows information regarding the production process. Data pertaining to heating and cooling are given in Table 3.6, while data pertaining to the washing of RR1 and RR2 are given in Table 3.7.

The objective in this case study was to determine the minimum makespan required to produce 200 kg each of Prod 1 and Prod 2, while also minimising external utility and freshwater consumption.

It is important to note the following from the data in Table 3.5, Table 3.6 and Table 3.7:

1. The processing duration of a batch is dependent on the batch size.
2. The mass load of contaminants is not fixed, but is dependent on the batch size.
3. The energy requirements of the operations are a function of the batch size and the given initial and final temperatures. Due to this fact, careful consideration must be given to ensure that whenever heat integration occurs between two operations, the minimum temperature difference for heat transfer, 10°C, is not violated.

Table 3.5. Data pertaining to production, for case study II.

Task (*i*)	Unit (*j*)	Max batch size (kg)	α_{ij} (h)	β_{ij} (h)	Washing time (h)	Material state	Initial inventory (kg)	Max storage (kg)	Revenue/ cost ($/kg or $/MJ)
Heating (H)	HR	100	0.667	0.007	0	Feed A (s1)	1000	1000	10
Reaction 1 (R1)	RR1	50	1.084	0.027	0.25	Feed B (s2)	1000	1000	10
	RR2	80	1.034	0.017	0.3	Feed C (s3/s4)	1000	1000	10
Reaction 2 (R2)	RR1	50	1.09	0.027	0.25	Hot A (s5)	0	100	0
	RR2	80	1.034	0.017	0.3	Int AB (s8)	0	200	0
Reaction 3 (R3)	RR1	50	0.417	0.013	0.25	Int BC (s6)	0	150	0
	RR2	80	0.367	0.008	0.3	Impure E (s9)	0	200	0
Separation (S)	SR	200	1.334	0.007	0	Prod 1 (s7)	0	1000	20
						Prod 2 (s10)	0	1000	20
						Washwater			0.1
						Wastewater			0.05
						Cooling water			0.02
						Steam			1

Table 3.6. Data pertaining to energy requirements, for case study II.

Task (*i*)	T_{in} (°C)	T_{out} (°C)	Unit (*j*)	cp (kJ/kg°C)
Heating (H)	50	70	HR	2.5
Reaction 1 (R1)	100	70	RR1	3.5
			RR2	3.5
Reaction 2 (R2)	70	100	RR1	3.2
			RR2	3.2
Reaction 3 (R3)	100	130	RR1	2.6
			RR2	2.6
Separation (S)	130	100	SR	2.8
Cooling water	20	30		
Steam	170	160		

Table 3.7. Data pertaining to water requirements, for case study II.

Task (*i*)	Unit (*j*)	Max inlet concentration (ppm)				Max outlet concentration (ppm)				Contaminant loading (g contaminant/kg batch)
		ar	br	cp	dw	ar	br	cp	dw	
Reaction 1 (R1)	RR1	300	500	800	400	700	800	1200	900	0.2
	RR2	300	500	800	400	700	800	1200	900	0.2
Reaction 2 (R2)	RR1	700	600	300	400	1200	1000	600	800	0.2
	RR2	700	600	300	400	1200	1000	600	800	0.2
Reaction 3 (R3)	RR1	500	200	400	300	800	500	700	900	0.2
	RR2	500	200	400	300	800	500	700	900	0.2

The second case study was solved using the proposed formulation, using Constraints (3.1), (3.2), (3.17) to (3.23), (3.26) to (3.35), (3.40) to (3.43), (3.45) to (3.50), (3.52), (3.60) to (3.69) and (3.85) to (3.88). The objective function was the minimisation of makespan, Constraint (3.92). It is important to note that in Constraints (3.40), (3.41), (3.43) and (3.45), variables associated with wastewater storage are not included. This is in order to make a direct comparison with the results obtained by Halim and Srinivasan (2011). The computer used to solve the model had an Intel(R) Core(TM) i7-2670QM, 2.2 GHz processor with 4.0 GB RAM. The problem was solved with GAMS using DICOPT for the MINLP with CPLEX as the MIP solver and MINOS as the NLP solver.

Figure 3.6 shows the Gantt chart with the resulting production schedule for the case study. The clear horizontal blocks represent the tasks associated with production processes. The amount of material processed in each unit is labelled within the clear blocks. The dark horizontal blocks represent the washing of a unit. The amount of water associated with washing is labelled underneath the relevant dark blocks. The double sided arrows (up-down arrows) represent direct heat integration between two tasks. The numbers in round brackets represent the amount of energy associated with heat integration. The numbers in curly brackets represent steam duties while the numbers in square brackets represent cooling water duties.

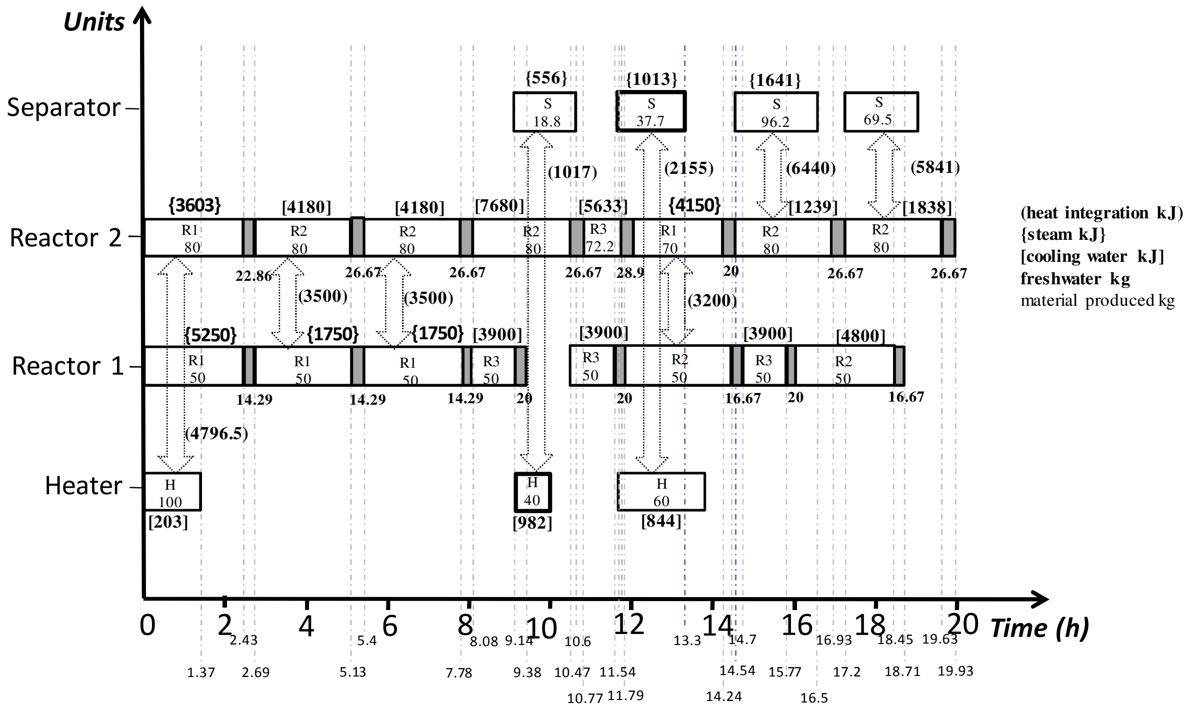

Figure 3.6. Resulting production schedule for case study II.

A comparison between the results of this case study obtained by Halim and Srinivasan (2011) and the proposed formulation is described in Table 3.8.

As can be observed from Table 3.8, improved objectives were obtained using the proposed formulation with the exception of the amount of freshwater used for washing. This was probably due to the fact that the cost associated with using steam was more significant than the cost associated with using freshwater. Hence, to minimise overall costs, promoting opportunities for heat integration took precedence over promoting opportunities for water reuse. This can be observed from the production schedule in Figure 3.6. With the operations aligned to promote heat integration, no opportunities for water reuse exist at all.

Table 3.8. Comparison of results for case study II.

	Halim & Srinivasan (2011)	This formulation
Makespan (h)	19.96	19.93
Steam (MJ)	61.36	44.88
Cooling water (MJ)	35.39	19.72
Total freshwater (kg)	275.09	341.2
Revenue from products ($)	8000	8000
Cost of raw materials ($)	5604.4	5444.4
Cost of steam ($)	61.36	44.88
Cost of cooling water ($)	0.7078	0.3994
Cost of freshwater ($)	27.509	34.12
Cost of wastewater ($)	13.75	17.06
Profit ($)	2292.3	2459.1
Number of slots	8	N/A
Number of time points	N/A	17
Number of iterations	3500	N/A
CPU time (s)	not reported	24 532
Number of binary variables	not reported	836
Major iterations	-	9

The MINLP model was solved by the aforementioned initialisation procedure. The objective value from the relaxed MINLP model was 123.543 $/h and the objective value from the exact MINLP model was 123.369 $/h. As both the relaxed model and exact models were MINLP, due to the nonlinear objective function, the global optimality of the solution could not be guaranteed.

3.7 Case study III

This case study was obtained from Majozi and Gouws (2009) and was extended to include heat integration opportunities. The multipurpose batch facility investigated, is similar to that discussed in Case Study II. The heating and separation tasks performed in HR and SR, respectively, are not to be heat integrated with any other units. Heat integration can only occur between RR1 and RR2 depending on the tasks they perform. Similarly, water is required for washing RR1 and RR2 at the end of any reaction. In this case study, three contaminants, C1, C2 and C3 are present. Table 3.9 shows information regarding the production process, while data pertaining to the washing of RR1 and RR2, obtained from Majozi and Gouws (2009) are given in Table 3.10. The heat integration data are provided in Table 3.11.

Table 3.9. Production data for case study III.

Task (*i*)	Unit (*j*)	Max batch size (kg)	Mean processing time (h)	Washing time (h)	Material state	Initial inventory (kg)	Max storage (kg)	Revenue/cost (c.u./kg or c.u./kJ)
Heating (H)	HR	100	1	0	Feed A (s1)	Unlimited	Unlimited	0
Reaction 1 (R1)	RR1	50	2	0.25	Feed B (s2)	Unlimited	Unlimited	0
	RR2	80	2	0.3	Feed C (s3/s4)	Unlimited	Unlimited	0
Reaction 2 (R2)	RR1	50	2	0.5	Hot A (s5)	0	0	0
	RR2	80	2	0.25	Int AB (s8)	0	0	0
Reaction 3 (R3)	RR1	50	1	0.25	Int BC (s6)	0	0	0
	RR2	80	1	0.25	Impure E (s9)	0	0	0
Separation (S)	SR	200	1 for Prod 2,	0	Prod 1 (s7)	0	0	100
			2 for Int AB		Prod 2 (s10)	0	0	100
					Washwater			2
					Wastewater			3
					Cooling water			2
					Steam			10

Table 3.10. Wastewater minimisation data for case study III.

		Maximum contaminant concentration (g contaminant/kg water)		
		C1	C2	C3
Reaction 1 (RR1)	Max. inlet	0.5	0.5	2.3
	Max. outlet	1	0.9	3
Reaction 2 (RR1)	Max. inlet	0.01	0.05	0.3
	Max. outlet	0.2	0.1	1.2
Reaction 3 (RR1)	Max. inlet	0.15	0.2	0.35
	Max. outlet	0.3	1	1.2
Reaction 1 (RR2)	Max. inlet	0.05	0.2	0.05
	Max. outlet	0.1	1	12
Reaction 2 (RR2)	Max. inlet	0.03	0.1	0.2
	Max. outlet	0.075	0.2	1
Reaction 3 (RR2)	Max. inlet	0.3	0.6	1.5
	Max. outlet	2	1.5	2.5
		Contaminant mass load (g)		
		C1	C2	C3
Reaction 1	Reactor 1	4	80	10
	Reactor 2	15	24	358
Reaction 2	Reactor 1	28.5	7.5	135
	Reactor 2	9	2	16
Reaction 3	Reactor 1	15	80	85
	Reactor 2	22.5	45	36.5

In this case study, storage facilities for heat storage and water reuse are available. Different scenarios of the case study were solved to demonstrate the capabilities of the model. These scenarios are as follows:

- Scenario 1: During production, only freshwater is available for washing. Heating and cooling are provided exclusively by steam and cooling water.
- Scenario 2: In addition to freshwater for washing, steam for heating and cooling water for cooling, opportunities for direct water reuse and direct heat integration are explored.

- Scenario 3: The effect of the inclusion of storage facilities for heat and wastewater (indirect heat integration and indirect water reuse) to Scenario 2 is explored.

Table 3.11. Heat integration data for case study III.

Reaction	Type	Heating/cooling requirement (kWh)	Operating Temperature (°C)
RX1	exothermic	60 (cooling)	100
RX2	endothermic	80 (heating)	60
RX3	exothermic	70 (cooling)	140

Heat storage parameters	Values
cp_{fluid} (kJ/kg°C)	4.2
$\Delta T^{\min}$ (°C)	10
T^{L} (°C)	20
T^{U} (°C)	180
W^{L} (ton)	1
W^{U} (ton)	3

Constraints (3.1) to (3.16), (3.24) to (3.25), (3.34) to (3.39), (3.40) to (3.43), (3.44) and (3.47) to (3.91) were used to solve this case study. The bilinear terms present in the model were linearised and the solution procedure as described above was used.

The capacity of the storage vessel for water was 200 kg. The objective of this case study was to maximise profit while minimising energy consumption and wastewater production, within a time horizon of 12 h. The storage capacity and the initial temperature of the heat storage vessel were variables to be optimised (Stamp & Majozi, 2011). Heat losses were not considered.

The computer used to solve the model had an Intel(R) Core(TM) i7-2670QM, 2.2 GHz processor with 4.0 GB RAM. The problem was solved with GAMS using DICOPT for the

MINLP with CPLEX as the MIP solver and CONOPT as the NLP solver. A comparison between the three scenarios is provided in Table 3.12. The results of Scenario 1, Scenario 2 and Scenario 3 are contained in column 2, 3 and 4, respectively, of Table 3.12.

Table 3.12. Comparison between different scenarios for case study III.

	Freshwater and utilities	Direct water reuse and direct heat integration	Direct/indirect water reuse and direct/indirect heat integration
Profit (c.u.)	18 537	19 836	22 235
Amount of Prod 1 (kg)	96	116	116
Amount of Prod 2 (kg)	162	156.4	188
Cooling water (kWh)	390	250	190
Steam (kWh)	240	180	10
Freshwater (kg)	816	1 020	896
Time points	11	11	13
CPU time (s)	3.1	14.8	42 275
Binary variables	128	508	954
Initial storage temperature (°C)			82.9
Heat storage capacity (ton)			2.024
Major iterations	3	3	4

From Table 3.12 it can be observed that profit increases from Scenario 1 to Scenario 3, with a decrease in steam and cooling water requirements. However, while cooling water and steam decreased in Scenario 2 compared to Scenario 1, the amount of freshwater increased. The total amount of product in Scenario 1 is 258 kg, while the total amount of product in Scenario 2 is 272.4 kg. This is as a result of additional unit operations being performed in Scenario 2 than are performed in Scenario 1. These additional unit operations contribute to the increased amount of washing water required. Furthermore, no opportunities for direct water reuse were realised due to the cost of steam relative to the cost of freshwater. The unit operations are aligned in such a way as to promote as much heat integration as possible. In so doing, opportunities for direct water reuse are lost. In Scenario 3, storage for water is available and hence a decrease is observed in the amount of freshwater used. The resulting process schedule for the results of Scenario 2 is illustrated in Figure 3.7, while the corresponding schedule for Scenario 3 is illustrated in Figure 3.8.

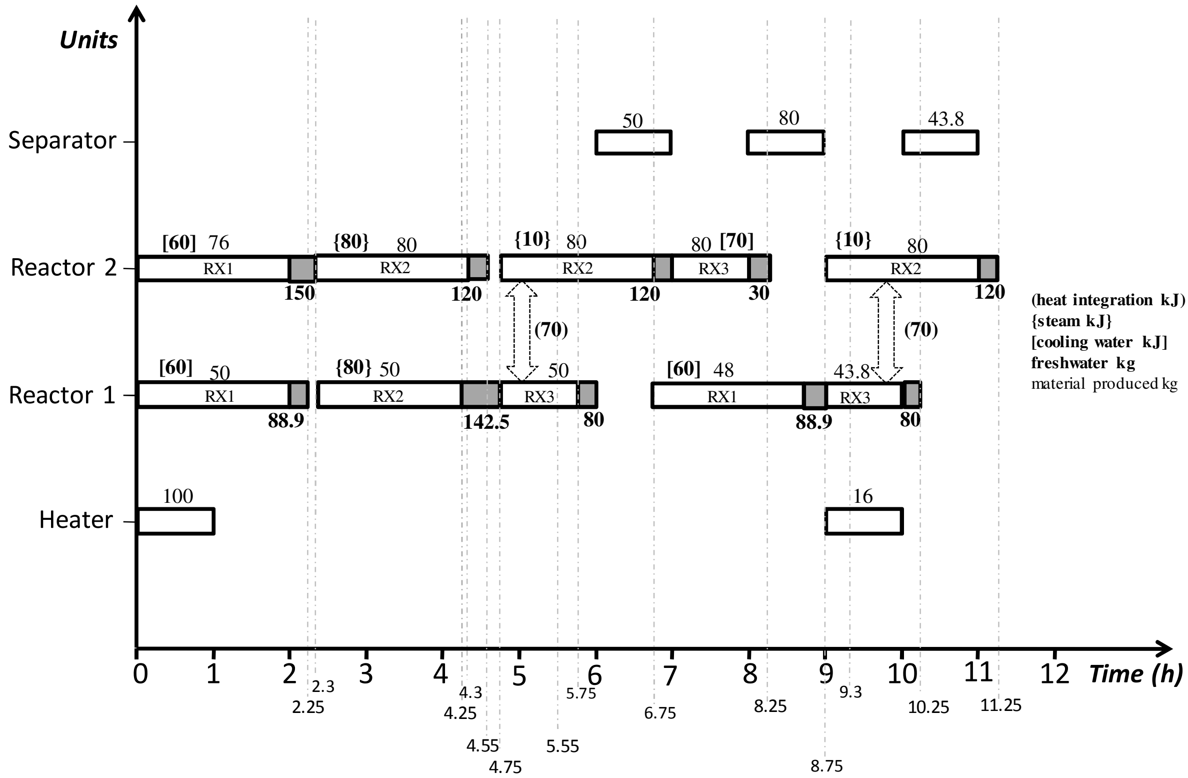

Figure 3.7. Resulting process schedule when only direct heat integration and direct water reuse are possible.

The clear blocks represent the production operation in the unit while the dark blocks represent the washing operations which take place after the reactions are completed. The numbers above the clear blocks represent the amount of material processed in the unit during production and the numbers below the washing operations represent freshwater. Water transfer to and from storage has been clearly labelled. The up-down arrows represent direct heat integration, while the bent arrows represent indirect heat integration to or from the heat storage unit. The results of Scenario 1 are globally optimal with the objective function of the linearised MILP and exact MINLP being 18 537 c.u. Similarly, the results of Scenario 2 are globally optimal, with the objective function of the linearised MILP and exact MINLP being 19 836 c.u. In Scenario 3, the objective function of the linearised MILP was 25 270 c.u., while the objective function of the exact MINLP was 22 235 c.u. Hence, the results for Scenario 3 are locally optimal.

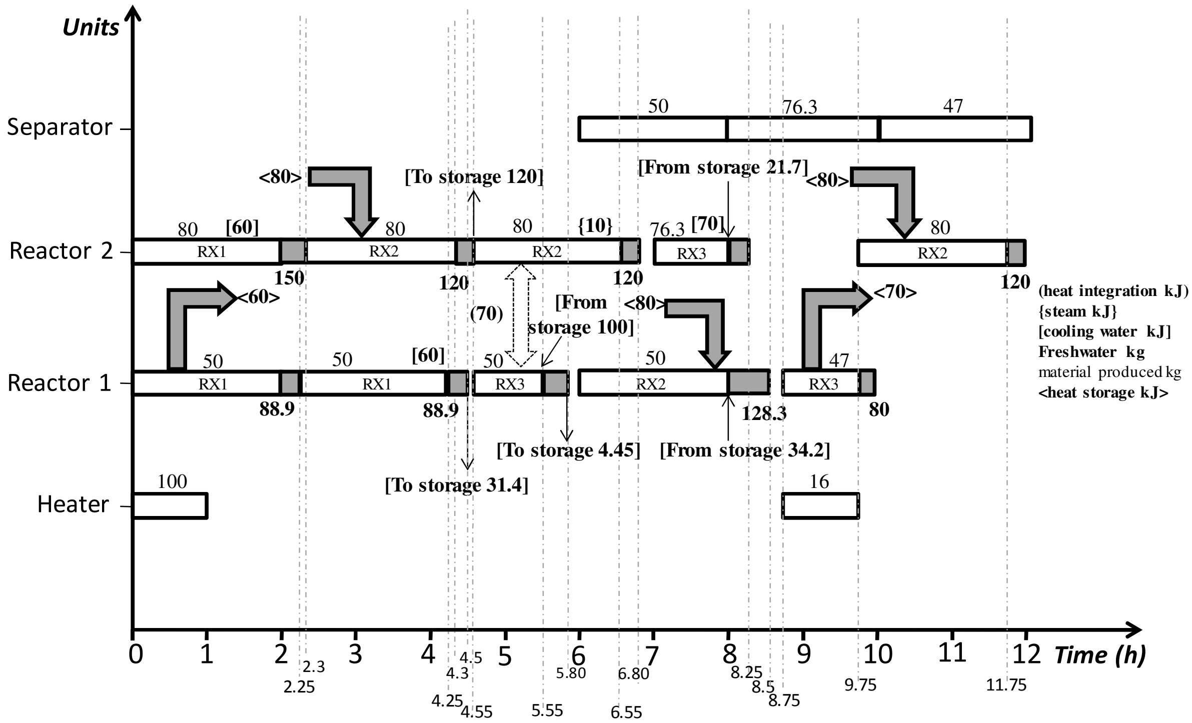

Figure 3.8. Resulting process schedule when both direct/indirect heat integration and wastewater minimisation are possible.

3.8 Conclusions

A simultaneous method for the optimisation of energy and water embedded within a scheduling framework has been developed. Furthermore, opportunities for direct and indirect heat integration as well as direct and indirect water reuse have been explored. The mathematical formulation led to a MINLP problem for which an initialisation procedure was employed.

The applicability of the method has been demonstrated with three case studies. The developed formulation has proved to effectively solve a complex makespan minimisation problem in which duration is a function of batch size and which included multiple contaminants, achieving an improved profit of 6.78% compared to a published sequential method.

The advantage of the developed model is that the variable nature of time ensures that the schedule is flexible and results that could have been overlooked when time is fixed are available during the optimisation search, leading to better overall objectives. The problem could in future also be extended to include water using operations other than equipment washing.

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CHAPTER 4

LONG-TERM HEAT INTEGRATION

4.1 Introduction

Most scheduling methods are limited to the short-term scheduling case and solution of problems over long time horizons may prove challenging or impossible with these current methods. Including additional considerations such as heat integration further complicates the problem. Cyclic scheduling methods may be preferred in order to obtain a feasible solution where a solution with short-term methods might not be possible or feasible otherwise.

The method of Stamp and Majozi (2011) has been extended to solve heat integration problems over long time horizons. The method uses the cyclic scheduling concepts and solution procedure presented by Wu and Ierapetritou (2004). These concepts were also used in a similar technique in the solution of long-term wastewater minimisation problems in multipurpose batch plants by Nonyane and Majozi (2012). Consideration of both the start-up and finishing periods is also included. The cyclic scheduling method results in obtaining a feasible solution over a shorter time horizon in improved computational time. The cyclic scheduling model can also be used for extended time horizons as the time horizon does not affect the computational complexity in solving the model.

The proposed method includes the concept of indirect heat integration via heat storage, rather than just direct heat integration. This has not been considered in long-term heat integration models in current literature. The initial heat storage temperature and the heat storage capacity are also optimised. The heat integration model of Stamp and Majozi (2011) and the cyclic scheduling constraints of Wu and Ierapetritou (2004) have been embedded into the scheduling model of Seid and Majozi (2012), which has shown to result in improvements in computational time as well as objective function in short-term scheduling problems.

The complete cyclic scheduling model is useful for the simultaneous optimisation of the schedule and energy usage for multipurpose batch plants operated over a long time horizon and was applied to two literature examples and an industrial case study.

4.2 Cyclic scheduling concepts

Shah *et al.* (1993) proposed an axiom which stated that, in the case where the time horizon of interest is much longer than the individual task durations, there exists a sub-schedule of much shorter duration which, when repeated, can achieve production close to the optimal production achievable for the original long time horizon. This was the basis for the development of cyclic scheduling techniques. It involves obtaining an optimal cyclic schedule which is then repeated and this therefore reduces the problem size. Although cyclic scheduling sacrifices some accuracy when compared to the direct solution of the scheduling problem, this is balanced by the easier and quicker solution of a less complex scheduling problem.

In the cyclic scheduling approach, the length of the cycle is an optimisation variable. The unit schedule is then also optimised. For the unit schedule to be repeatable, a certain amount of each intermediate state must be available to start the cyclic period. It is also required that the intermediates be produced and stored at the end of the period to be available for the next period. In cyclic scheduling, each unit has an individual cycle with cycle time equal to the unit period cycle duration. The units therefore do not need to share the same starting and ending times. This leads to the concept of the "wrapping around" of tasks as proposed by Shah *et al*. (1993) which allows tasks to cross a unit schedule boundary for improved unit utilisation. This concept is demonstrated in Figure 4.1 and Figure 4.2. The cyclic scheduling model of Wu and Ierapetritou (2004) was based on the previous discrete time model of Shah *et al*. (1993) and uses the continuous time scheduling constraints of Ierapetritou and Floudas (1998), based on the STN representation.

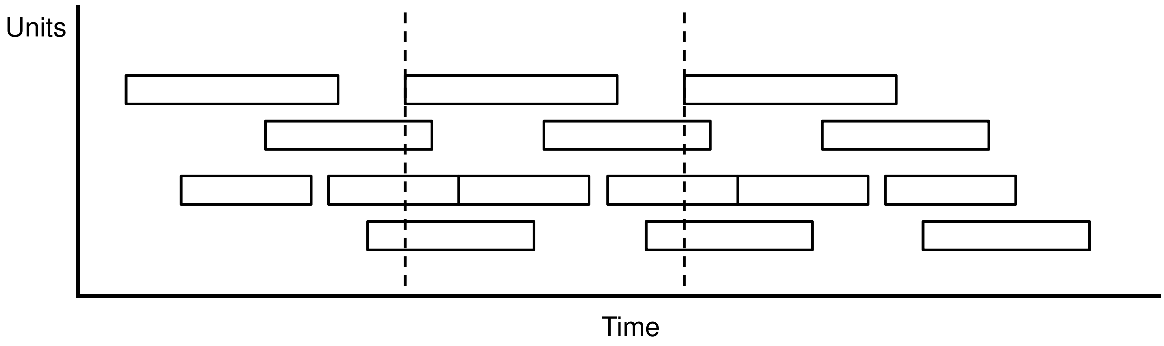

Figure 4.1. Representation of a cyclic schedule (Wu & Ierapetritou, 2004).

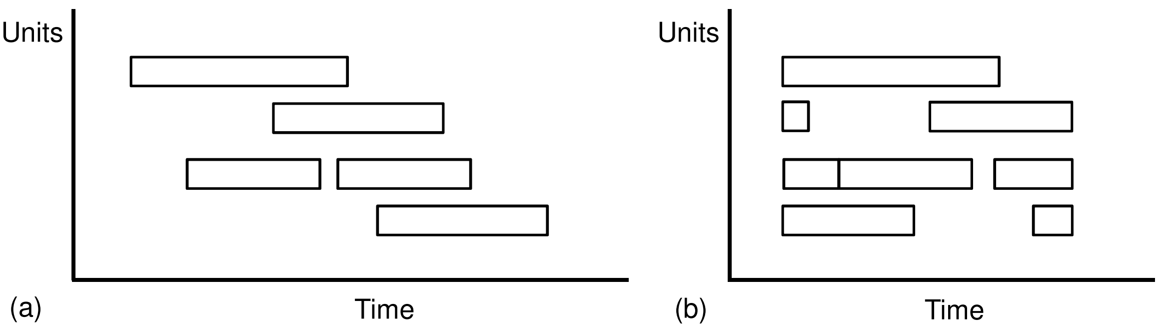

Figure 4.2. (a) Unit schedule (b) With tasks wrapping around (Wu & Ierapetritou, 2004).

The overall long time horizon is divided into three periods (Wu & Ierapetritou, 2004). The optimal unit schedule with optimal cycle length is solved for first, where the objective is to maximise the average profit over the cycle. This is the main period which will be repeated. Sub-ranges for the cycle time may be used rather than considering the entire cycle time at once. As the cycle time is a variable, this makes it easier to determine the required number of time points. These sub-problems may also be solved in parallel and generate alternative schedules with different cycle lengths which may be useful depending on the application.

The initial period, the start-up phase, is then solved. The results from this period ensure that the intermediates required to start the cyclic period are produced. The first objective is to minimise the makespan which ensures there is a feasible solution and the required intermediates are produced in the shortest possible time. The problem is then solved to maximise profit over the time horizon obtained from the makespan minimisation problem.

A profit maximisation problem is then solved for the final period, which is the remainder of the long time horizon. The final period, or shut-down phase, uses up all the remaining intermediates to form products. The initial and final period profit maximisation problems are both MILP short-term scheduling problems with known time horizons. The combined lengths of the three different periods add up to the overall long time horizon.

This method can easily be applied to any long time horizon as the initial period is not affected by the overall length of the time horizon considered. The number of cycles can be increased or decreased and the final period solved for again if the overall time horizon changes. The solution procedure and computational complexity are also not affected by a change in the overall time horizon. The method provides another option for the solution of long-term scheduling problems rather than solving them directly with short-term scheduling methods and its usefulness will therefore depend on the application.

4.3 Problem statement and objectives

The problem can be stated as follows:

Given:

Scheduling data

(i) production recipe for each product

(ii) available units and their capacities

(iii) maximum storage capacity for each material
(iv) task durations
(v) time horizon of interest
(vi) costs of raw materials
(vii) selling price of final products

Heat integration data

(i) hot duties for tasks requiring heating and cold duties for tasks that require cooling
(ii) operating temperatures of heat sources and heat sinks
(iii) minimum allowable temperature differences
(iv) heat capacities of materials
(v) costs of hot and cold utilities
(vi) design limits on heat storage

The objectives are then to determine the optimum cycle time and cyclic operating schedule as well as the schedules for the initial and final periods in order to optimise the profit over the given long time horizon.

4.4 Mathematical model

The mathematical model consists of the necessary scheduling constraints, heat integration constraints and cyclic scheduling constraints. The short-term scheduling model of Seid and Majozi (2012) was used and these constraints can be found in Appendix B. The heat integration constraints of Stamp and Majozi (2011) are the same as those used in the model in Section 3.3 of Chapter 3, but are repeated here for completeness. The cyclic scheduling constraints are discussed thereafter. The heat integration model is based on the superstructure in Figure 4.3 and includes opportunities for both direct and indirect heat integration. The complete model is useful for heat integrated multipurpose batch plants operated over long time horizons.

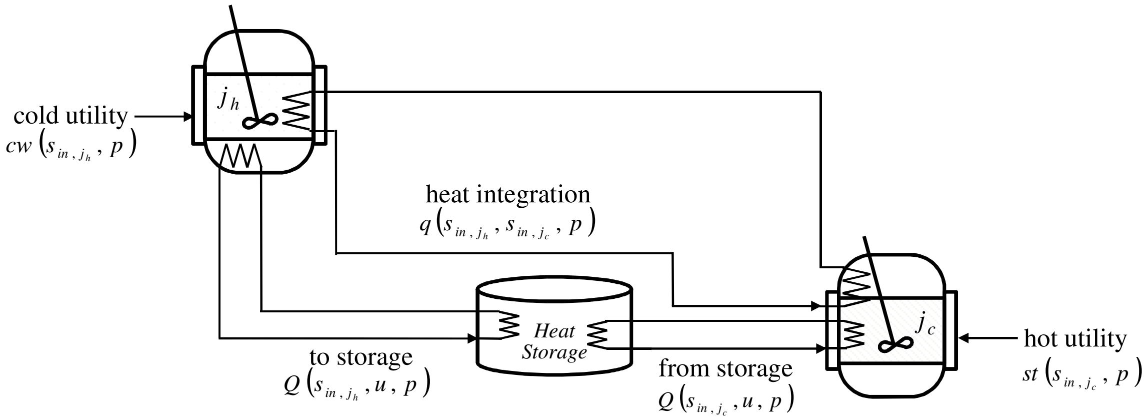

Figure 4.3. Superstructure for mathematical formulation when units perform heating/cooling tasks.

Each processing unit may operate using either direct or indirect heat integration. Direct heat integration refers to the use of heat generated from a processing unit to supply a processing unit requiring heat, without use of heat storage. Indirect heat integration refers to the use of heat previously stored in a heat storage vessel to supply a processing unit requiring heat. Processing units may also operate in standalone mode, using only external utilities. This may be required for control reasons or when thermal driving forces or time do not allow for heat integration. If either direct or indirect heat integration is not sufficient to satisfy the required duty, external utilities may make up for any deficit.

Constraints (4.1) and (4.2) are active simultaneously and ensure that one hot unit will be integrated with one cold unit when direct heat integration takes place, in order to simplify operation of the process. Also, if two units are to be heat integrated at a given time point, they must both be active at that time point. However, if a unit is active, it may operate in either integrated or standalone mode.

$$\sum_{s_{in,j_c}} x\left(s_{in,j_c}, s_{in,j_h}, p\right) \leq y\left(s_{in,j_h}, p\right), \qquad \forall\ p \in P,\quad s_{in,j_h} \in S_{in,j} \tag{4.1}$$

$$\sum_{s_{in,j_h}} x\left(s_{in,j_c}, s_{in,j_h}, p\right) \leq y\left(s_{in,j_c}, p\right), \qquad \forall\ p \in P,\quad s_{in,j_c} \in S_{in,j} \tag{4.2}$$

Constraints (4.3) and (4.4) ensure that heat integration between a unit and heat storage may occur only if the unit is active at that time point. However, if a unit is active, it will not necessarily integrate with heat storage.

$$z\left(s_{in,j_c}, u, p\right) \leq y\left(s_{in,j_c}, p\right), \qquad \forall\ p \in P,\quad s_{in,j_c} \in S_{in,j},\quad u \in U \tag{4.3}$$

$$z\left(s_{in,j_h}, u, p\right) \leq y\left(s_{in,j_h}, p\right), \qquad \forall\ p \in P,\quad s_{in,j_h} \in S_{in,j},\quad u \in U \tag{4.4}$$

Constraint (4.5) ensures that heat storage is heat integrated with either one hot unit or one cold unit at any point in time. This is to simplify and improve operational efficiency in the plant.

$$\sum_{s_{in,j_c}} z\left(s_{in,j_c}, u, p\right) + \sum_{s_{in,j_h}} z\left(s_{in,j_h}, u, p\right) \leq 1, \qquad \forall\ p \in P,\quad u \in U \tag{4.5}$$

Constraints (4.6) and (4.7) ensure that a unit cannot simultaneously undergo direct and indirect heat integration. This condition simplifies the operation of the process.

$$\sum_{s_{in,j_h}} x\left(s_{in,j_c}, s_{in,j_h}, p\right) + z\left(s_{in,j_c}, u, p\right) \leq 1, \qquad \forall\ p \in P,\quad s_{in,j_c} \in S_{in,j},\quad u \in U \tag{4.6}$$

$$\sum_{s_{in,j_c}} x\left(s_{in,j_c}, s_{in,j_h}, p\right) + z\left(s_{in,j_h}, u, p\right) \leq 1, \qquad \forall\ p \in P,\quad s_{in,j_h} \in S_{in,j},\quad u \in U \tag{4.7}$$

Constraints (4.8) and (4.9) quantify the amount of heat received from or transferred to the heat storage unit, respectively. There will be no heat received or transferred if the binary variable signifying usage of the heat storage vessel, $z\left(s_{in,j}, u, p\right)$, is zero. These constraints are active over the entire time horizon, where p is the current time point and $p-1$ is the previous time point.

$$Q\left(s_{in,j_c},u,p-1\right)=W(u)cp_{fluid}\left(T_0(u,p-1)-T_f(u,p)\right)z\left(s_{in,j_c},u,p-1\right),$$
$$\forall\ p\in P, p>p0,\quad s_{in,j_c}\in S_{in,j},\quad u\in U \tag{4.8}$$

$$Q\left(s_{in,j_h},u,p-1\right)=W(u)cp_{fluid}\left(T_f(u,p)-T_0(u,p-1)\right)z\left(s_{in,j_h},u,p-1\right),$$
$$\forall\ p\in P, p>p0,\quad s_{in,j_h}\in S_{in,j},\quad u\in U \tag{4.9}$$

Constraint (4.10) quantifies the heat transferred to the heat storage vessel at the beginning of the time horizon. The initial temperature of the heat storage fluid is $T_0(u,p0)$.

$$Q\left(s_{in,j_h},u,p0\right)=W(u)cp_{fluid}\left(T_f(u,p1)-T_0(u,p0)\right)z\left(s_{in,j_h},u,p0\right),$$
$$\forall\ s_{in,j_h}\in S_{in,j},\quad u\in U \tag{4.10}$$

Constraint (4.11) ensures that the final temperature of the heat storage fluid at any time point becomes the initial temperature of the heat storage fluid at the next time point. This condition will hold regardless of whether or not there was heat integration at the previous time point.

$$T_0(u,p)=T_f(u,p-1),\qquad \forall\ p\in P,\quad u\in U \tag{4.11}$$

Constraints (4.12) and (4.13) ensure that the temperature of heat storage does not change if there is no heat integration with the heat storage unit, unless there is heat loss from the heat storage unit. MM is any large number, thereby resulting in an overall "Big M" formulation. If either $z\left(s_{in,j_c},u,p-1\right)$ or $z\left(s_{in,j_h},u,p-1\right)$ is equal to one, Constraint (4.12) and Constraint (4.13) will be redundant. However, if these two binary variables are both zero, the initial temperature at the previous time point will be equal to the final temperature at the current time point.

$$T_0(u,p-1) \le T_f(u,p) + MM\left(\sum_{s_{in,j_c}} z(s_{in,j_c},u,p-1) + \sum_{s_{in,j_h}} z(s_{in,j_h},u,p-1)\right),$$
$$\forall\ p \in P, p > p0,\quad u \in U \tag{4.12}$$

$$T_0(u,p-1) \ge T_f(u,p) - MM\left(\sum_{s_{in,j_c}} z(s_{in,j_c},u,p-1) + \sum_{s_{in,j_h}} z(s_{in,j_h},u,p-1)\right),$$
$$\forall\ p \in P, p > p0,\quad u \in U \tag{4.13}$$

Constraint (4.14) ensures that minimum thermal driving forces are obeyed when there is direct heat integration between a hot and a cold unit. This constraint holds when both hot and cold units operate at constant temperature, which is commonly encountered in practice. An example is when there is heat integration between an exothermic and an endothermic reaction.

$$T(s_{in,j_h}) - T(s_{in,j_c}) \ge \Delta T^{\min} - MM\left(1 - x(s_{in,j_c}, s_{in,j_h}, p-1)\right),$$
$$\forall\ p \in P, p > p0,\quad s_{in,j_c}, s_{in,j_h} \in S_{in,j} \tag{4.14}$$

Constraints (4.15) and (4.16) ensure that minimum thermal driving forces are obeyed when there is heat integration with the heat storage unit. Constraint (4.15) applies for heat integration between heat storage and a heat sink, while constraint (4.16) applies for heat integration between heat storage and a heat source. In Constraints (4.15) and (4.16), the units operate at fixed temperatures. For units not operating at fixed temperatures, both inlet and outlet minimal thermal driving forces between the two integrated tasks need also to be enforced.

$$T_f(u,p) - T(s_{in,j_c}) \ge \Delta T^{\min} - MM\left(1 - z(s_{in,j_c}, u, p-1)\right),$$
$$\forall\ p \in P, p > p0,\quad s_{in,j_c} \in S_{in,j},\quad u \in U \tag{4.15}$$

$$T\left(s_{in,j_h}\right) - T_f(u,p) \geq \Delta T^{\min} - MM\left(1 - z\left(s_{in,j_h}, u, p-1\right)\right),$$
$$\forall\ p \in P, p > p0,\ s_{in,j_h} \in S_{in,j},\quad u \in U \tag{4.16}$$

Constraints (4.17) and (4.18) give the heating load for a cold state and cooling load for a hot state, respectively, for variable batch size and changing temperature.

$$HL\left(s_{in,j_c}, p\right) = B\left(s_{in,j_c}, p\right) cp_{state}\left(s_{in,j_c}\right)\left(T_{out}\left(s_{in,j_c}\right) - T_{in}\left(s_{in,j_c}\right)\right),$$
$$\forall\ p \in P,\quad s_{in,j_c} \in S_{in,j} \tag{4.17}$$

$$CL\left(s_{in,j_h}, p\right) = B\left(s_{in,j_h}, p\right) cp_{state}\left(s_{in,j_h}\right)\left(T_{in}\left(s_{in,j_h}\right) - T_{out}\left(s_{in,j_h}\right)\right),$$
$$\forall\ p \in P,\quad s_{in,j_h} \in S_{in,j} \tag{4.18}$$

Constraint (4.19) ensures that the heating of a cold state will be satisfied by either direct or indirect heat integration as well as external utility if required.

$$HL\left(s_{in,j_c}, p\right) = Q\left(s_{in,j_c}, u, p\right) + st\left(s_{in,j_c}, p\right) + \sum_{s_{in,j_h}} q\left(s_{in,j_c}, s_{in,j_h}, p\right),$$
$$\forall\ p \in P,\quad s_{in,j_c} \in S_{in,j},\quad u \in U \tag{4.19}$$

Constraint (4.20) states that the cooling of a hot state will be satisfied by either direct or indirect heat integration as well as external utility if required.

$$CL\left(s_{in,j_h}, p\right) = Q\left(s_{in,j_h}, u, p\right) + cw\left(s_{in,j_h}, p\right) + \sum_{s_{in,j_c}} q\left(s_{in,j_c}, s_{in,j_h}, p\right),$$
$$\forall\ p \in P,\quad s_{in,j_h} \in S_{in,j},\quad u \in U \tag{4.20}$$

The upper bounds of the heating load of a cold state, the cooling load of a hot state and the amount of heat exchanged during direct integration are given in Constraints (4.21) to (4.23).

$$HL\left(s_{in,j_c}, p\right) \le y\left(s_{in,j_c}, p\right) Q^{\max}\left(s_{in,j_c}\right), \qquad \forall\ p \in P, \quad s_{in,j_c} \in S_{in,j} \tag{4.21}$$

$$CL\left(s_{in,j_h}, p\right) \le y\left(s_{in,j_h}, p\right) Q^{\max}\left(s_{in,j_h}\right), \qquad \forall\ p \in P, \quad s_{in,j_h} \in S_{in,j} \tag{4.22}$$

$$q\left(s_{in,j_c}, s_{in,j_h}, p\right) \le x\left(s_{in,j_c}, s_{in,j_h}, p\right) \min\left\{Q^{\max}\left(s_{in,j_c}\right), Q^{\max}\left(s_{in,j_h}\right)\right\}$$
$$\forall\ p \in P, \quad s_{in,j_c}, s_{in,j_h} \in S_{in,j} \tag{4.23}$$

For the specific case where the heating and cooling loads are fixed, Constraints (4.24) and (4.25) are used instead of (4.19) and (4.20).

$$HL\left(s_{in,j_c}\right) y\left(s_{in,j_c}, p\right) = Q\left(s_{in,j_c}, u, p\right) + st\left(s_{in,j_c}, p\right)$$
$$+ x\left(s_{in,j_c}, s_{in,j_h}, p\right) \sum_{s_{in,j_h}} \min_{s_{in,j_c}, s_{in,j_h}} \left\{HL\left(s_{in,j_c}\right), CL\left(s_{in,j_h}\right)\right\},$$
$$\forall\ p \in P, \quad s_{in,j_c} \in S_{in,j}, \quad u \in U \tag{4.24}$$

$$CL\left(s_{in,j_h}\right) y\left(s_{in,j_h}, p\right) = Q\left(s_{in,j_h}, u, p\right) + cw\left(s_{in,j_h}, p\right)$$
$$+ x\left(s_{in,j_c}, s_{in,j_h}, p\right) \sum_{s_{in,j_c}} \min_{s_{in,j_c}, s_{in,j_h}} \left\{HL\left(s_{in,j_c}\right), CL\left(s_{in,j_h}\right)\right\},$$
$$\forall\ p \in P, \quad s_{in,j_h} \in S_{in,j}, \quad u \in U \tag{4.25}$$

The amount of heat transferred through direct heat integration will be limited by the smaller heating or cooling requirement of the heat integrated tasks. Constraints (4.26) and (4.27) express this. Constraint (4.26) calculates the heat load of the cold task, while Constraint (4.27) calculates the cooling load of the hot task.

$$q\left(s_{in,j_c}, s_{in,j_h}, p\right) \le B\left(s_{in,j_c}, p\right) cp_{state}\left(s_{in,j_c}\right)\left(T_{out}\left(s_{in,j_c}\right) - T_{in}\left(s_{in,j_c}\right)\right) x\left(s_{in,j_c}, s_{in,j_h}, p\right),$$
$$\forall\ p \in P, \quad s_{in,j_c}, s_{in,j_h} \in S_{in,j} \tag{4.26}$$

$$q\left(s_{in,j_c}, s_{in,j_h}, p\right) \leq B\left(s_{in,j_h}, p\right) cp_{state}\left(s_{in,j_h}\right)\left(T_{in}\left(s_{in,j_h}\right) - T_{out}\left(s_{in,j_h}\right)\right) x\left(s_{in,j_c}, s_{in,j_h}, p\right),$$
$$\forall\ p \in P,\quad s_{in,j_c}, s_{in,j_h} \in S_{in,j} \tag{4.27}$$

Furthermore, it is possible that a given pair of tasks cannot be heat integrated or that a possible $\Delta T^{\min}$ violation may occur. The possibility of heat integration between pairs of tasks as well as possible $\Delta T^{\min}$ violations should be investigated for each pair of hot and cold tasks beforehand. If $\Delta T^{\min}$ violations occur, the temperatures in Constraints (4.26) and (4.27) should be adjusted for this.

The amount of heat transferred through direct heat integration can also be limited by the duration of the shorter task if the tasks have different durations. Constraints (4.28) to (4.33) capture this. Constraints (4.28) and (4.29) calculate the heating load per time and cooling load per time, of the cold task and hot task, respectively.

$$\dot{HL}\left(s_{in,j_c}, p\right) = \frac{HL\left(s_{in,j_c}, p\right)}{dur\left(s_{in,j_c}, p\right)}, \qquad \forall\ p \in P,\quad s_{in,j_c} \in S_{in,j} \tag{4.28}$$

$$\dot{CL}\left(s_{in,j_h}, p\right) = \frac{CL\left(s_{in,j_h}, p\right)}{dur\left(s_{in,j_h}, p\right)}, \qquad \forall\ p \in P,\quad s_{in,j_h} \in S_{in,j} \tag{4.29}$$

Constraint (4.30) calculates the heat load of the cold task based on the duration of the same cold task. Constraint (4.31) calculates the heat load of the cold task based on the duration of the hot task. Constraint (4.32) calculates the cooling load of the hot task based on the duration of the same hot task. Constraint (4.33) calculates the cooling load of the hot task based on the duration of the cold task. The amount of heat integrated directly will effectively be the minimum of these four quantities.

$$q\left(s_{in,j_c}, s_{in,j_h}, p\right) \leq \dot{HL}\left(s_{in,j_c}, p\right) dur\left(s_{in,j_c}, p\right), \qquad \forall\ p \in P,\quad s_{in,j_c}, s_{in,j_h} \in S_{in,j} \tag{4.30}$$

$$q\left(s_{in,j_c}, s_{in,j_h}, p\right) \leq \dot{HL}\left(s_{in,j_c}, p\right) dur\left(s_{in,j_h}, p\right), \qquad \forall\ p \in P, \quad s_{in,j_c}, s_{in,j_h} \in S_{in,j} \tag{4.31}$$

$$q\left(s_{in,j_c}, s_{in,j_h}, p\right) \leq \dot{CL}\left(s_{in,j_h}, p\right) dur\left(s_{in,j_h}, p\right), \qquad \forall\ p \in P, \quad s_{in,j_c}, s_{in,j_h} \in S_{in,j} \tag{4.32}$$

$$q\left(s_{in,j_c}, s_{in,j_h}, p\right) \leq \dot{CL}\left(s_{in,j_h}, p\right) dur\left(s_{in,j_c}, p\right), \qquad \forall\ p \in P, \quad s_{in,j_c}, s_{in,j_h} \in S_{in,j} \tag{4.33}$$

In Constraints (4.28) to (4.33), the duration is a function of batch size. If the duration is fixed, $\tau\left(s_{in,j}\right)$ is used and these constraints are then linear.

Constraints (4.34) and (4.35) ensure that the times at which units are active are synchronised when direct heat integration takes place. Starting times for the tasks in the integrated units are the same. This constraint may be relaxed for operations requiring preheating or precooling and is dependent on the process.

$$t_u\left(s_{in,j_h}, p\right) \geq t_u\left(s_{in,j_c}, p\right) - MM\left(1 - x\left(s_{in,j_c}, s_{in,j_h}, p\right)\right)$$
$$\forall\ p \in P, \quad s_{in,j_c}, s_{in,j_h} \in S_{in,j} \tag{4.34}$$

$$t_u\left(s_{in,j_h}, p\right) \leq t_u\left(s_{in,j_c}, p\right) + MM\left(1 - x\left(s_{in,j_c}, s_{in,j_h}, p\right)\right)$$
$$\forall\ p \in P, \quad s_{in,j_c}, s_{in,j_h} \in S_{in,j} \tag{4.35}$$

Constraints (4.36) and (4.37) ensure that if indirect heat integration takes place, the time at which a heat storage unit starts either to transfer or receive heat will be equal to the time a unit is active.

$$t_u\left(s_{in,j}, p\right) \geq t_0\left(s_{in,j}, u, p\right) - MM\left(y\left(s_{in,j}, p\right) - z\left(s_{in,j}, u, p\right)\right)$$
$$\forall\ p \in P, \quad u \in U, \quad s_{in,j} \in S_{in,j} \tag{4.36}$$

$$t_u(s_{in,j}, p) \le t_0(s_{in,j}, u, p) + MM\left(y(s_{in,j}, p) - z(s_{in,j}, u, p)\right)$$
$$\forall\ p \in P,\quad u \in U,\quad s_{in,j} \in S_{in,j} \tag{4.37}$$

Constraints (4.38) and (4.39) state that the time when heat transfer to or from a heat storage unit is finished will coincide with the time the task transferring or receiving heat has finished processing.

$$t_u(s_{in,j}, p-1) + \tau(s_{in,j})y(s_{in,j}, p-1) \ge t_f(s_{in,j}, u, p)$$
$$- MM\left(y(s_{in,j}, p-1) - z(s_{in,j}, u, p-1)\right)$$
$$\forall\ p \in P, p > p0,\quad u \in U,\quad s_{in,j} \in S_{in,j} \tag{4.38}$$

$$t_u(s_{in,j}, p-1) + \tau(s_{in,j})y(s_{in,j}, p-1) \le t_f(s_{in,j}, u, p)$$
$$+ MM\left(y(s_{in,j}, p-1) - z(s_{in,j}, u, p-1)\right)$$
$$\forall\ p \in P, p > p0,\quad u \in U,\quad s_{in,j} \in S_{in,j} \tag{4.39}$$

Constraints (4.8), (4.9) and (4.10) have trilinear terms where a binary variable and two continuous variables are multiplied. Constraints (4.28) to (4.33) have bilinear terms where two continuous variables are multiplied. This results in a nonconvex MINLP formulation. The linearisation procedure for these constraints is demonstrated in Section 3.4 of Chapter 3.

The necessary constraints for determining the optimal cyclic schedule are now described. The scheduling model of Seid and Majozi (2012) was used. Some constraints were modified to accommodate cyclic scheduling and are shown in this section. The value for "Big M" in the cyclic scheduling constraints and heat integration constraints is the value of the upper bound of the cycle length, H^U.

Mass balance between two cycles

Constraint (4.40) ensures that the amount of intermediate state s stored at the end of a cycle is the same as that stored at the beginning of the cycle. There is therefore no accumulation or shortage of intermediate states when the cycle is repeated.

$$q_s(s,p) = Q_s^0(s), \qquad \forall s \in S, \quad s \neq product, feed, \quad p = |P| \tag{4.40}$$

Sequence constraints between cycles: Completion of previous tasks

Constraint (4.41) defines the relationship between the last task of the previous cycle and the first task of the current cycle when tasks occur in different units. This maintains continuity of tasks between cycles.

$$t_u\left(s_{in,j'}, p0\right) \geq t_p\left(s_{in,j}, p\right) - H^U\left(1 - y\left(s_{in,j}, p-2\right)\right) - H,$$
$$\forall j \in J, \quad p = |P|, \quad s_{in,j} \in S_{in,j}^{sp}, \quad s_{in,j'} \in S_{in,j'}^{sc} \tag{4.41}$$

Constraint (4.42) is similar to Constraint (4.41), but is applicable when intermediate state s is produced from one unit.

$$t_u\left(s_{in,j'}, p0\right) \geq t_p\left(s_{in,j}, p\right) - H^U\left(2 - y\left(s_{in,j}, p-1\right) - tt(j,p)\right) - H,$$
$$\forall j \in J, \quad p = |P|, \quad s_{in,j} \in S_{in,j}^{sp}, \quad s_{in,j'} \in S_{in,j}^{sc} \tag{4.42}$$

Constraint (4.43) ensures that units are available when the same task is performed in the same unit (the same state is used in the same unit). A state can only be used in a unit after all preceding tasks in the unit have been completed.

$$t_u(s_{in,j}, p0) \geq t_p(s_{in,j}, p) - H, \qquad \forall j \in J, \quad p = |P|, \quad s_{in,j} \in S^*_{in,j} \tag{4.43}$$

Constraint (4.44) is similar to Constraint (4.43), but pertains to different tasks being performed in the same unit (different states used in the same unit). A task can only start in a unit after all previous tasks in the unit are complete.

$$t_u(s_{in,j}, p0) \geq t_p(s'_{in,j}, p) - H,$$
$$\forall j \in J, \quad p = |P|, \quad s_{in,j} \neq s'_{in,j}, \quad s_{in,j}, s'_{in,j} \in S^*_{in,j} \tag{4.44}$$

Tightening constraints

This is the same constraint as in the scheduling model, but the time horizon is now the cycle length. Constraint (4.45) is used to tighten the model. The sum of the durations of all tasks in a unit must be within one cycle length.

$$\sum_{s_{in,j} \in S^*_{in,j}} \sum_{p} \left(\tau(s_{in,j}) y(s_{in,j}, p) + \beta(s_{in,j}) m_u(s_{in,j}, p) \right) \leq H,$$
$$\forall p \in P, \quad j \in J \tag{4.45}$$

Constraints (4.46) and (4.47) ensure processing tasks take place within two cycles.

$$t_u(s_{in,j}, p) \leq 2H, \qquad \forall s_{in,j} \in S_{in,j}, \quad p \in P, \quad j \in J \tag{4.46}$$

$$t_p(s_{in,j}, p) \leq 2H, \qquad \forall s_{in,j} \in S_{in,j}, \quad p \in P, \quad j \in J \tag{4.47}$$

Constraints (4.48) and (4.49) ensure that the times the heat storage unit is active are within two cycles.

$$t_0(s_{in,j}, u, p) \leq 2H, \qquad \forall s_{in,j} \in S_{in,j}, \quad p \in P, \quad j \in J, \quad u \in U \tag{4.48}$$

$$t_f(s_{in,j}, u, p) \leq 2H, \qquad \forall s_{in,j} \in S_{in,j}, \quad p \in P, \quad j \in J, \quad u \in U \tag{4.49}$$

Constraints (4.50) to (4.85) cater for the wrapping of the heat storage temperature and ensure the temperature in heat storage is the same at the beginning and end of the cycle in order for the cycle to be repeated.

Constraints (4.50) and (4.51) are defined, where T_{start} is the initial heat storage temperature at the beginning of the cycle and T_{end} is the heat storage temperature at the end of the cycle.

$$\Delta T_{cw} = T_{end} - T_{start} \tag{4.50}$$

$$\Delta T_{st} = T_{start} - T_{end} \tag{4.51}$$

If the heat storage temperature at the end of the cycle is higher than the temperature at the beginning of the cycle, cooling will be required to bring the storage temperature back to the starting temperature – essential for repetition of the cycle. ΔT_{cw} will then be positive. If the heat storage temperature at the end of the cycle is lower than the temperature at the beginning of the cycle, heating will be required and ΔT_{st} will be positive.

Constraint (4.52) is used if the heat storage temperature at the end of the cycle is too high and cooling is required to bring it back to the temperature at the beginning of the cycle. Constraint (4.53) is similar, but will be used if extra heating is required at the end of the cycle to bring the heat storage temperature back to the starting temperature.

$$extra\_cw(u) = W(u)\, cp_{fluid} \Delta T_{cw} x_{cw} \tag{4.52}$$

$$extra\_st(u) = W(u)\, cp_{fluid} \Delta T_{st} x_{st} \tag{4.53}$$

Both constraints (4.52) and (4.53) contain bilinear terms, where a continuous variable, ΔT_{cw} or ΔT_{st}, is multiplied by a binary variable, x_{cw} or x_{st}, respectively. These constraints are linearised using the Glover transformation (Glover, 1975). Constraint (4.52) is linearised using constraints (4.54) to (4.59) and Constraint (4.53) is linearised using Constraints (4.60) to (4.65). Constraints (4.66) and (4.67) are then obtained.

$$\Delta T_{cw} x_{cw} = G_{cw} \tag{4.54}$$

$$\Delta T^{L} \leq \Delta T_{cw} \leq \Delta T^{U} \tag{4.55}$$

$$G_{cw} \geq \Delta T_{cw} - \Delta T^{U}(1 - x_{cw}) \tag{4.56}$$

$$G_{cw} \leq \Delta T_{cw} + \Delta T^{L}(1 - x_{cw}) \tag{4.57}$$

$$G_{cw} \leq \Delta T^{U} x_{cw} \tag{4.58}$$

$$G_{cw} \geq \Delta T^{L} x_{cw} \tag{4.59}$$

$$\Delta T_{st} x_{st} = G_{st} \tag{4.60}$$

$$\Delta T^{L} \leq \Delta T_{st} \leq \Delta T^{U} \tag{4.61}$$

$$G_{st} \geq \Delta T_{st} - \Delta T^{U}(1 - x_{st}) \tag{4.62}$$

$$G_{st} \leq \Delta T_{st} + \Delta T^{L}(1 - x_{st}) \tag{4.63}$$

$$G_{st} \leq \Delta T^{U} x_{st} \tag{4.64}$$

$$G_{st} \geq \Delta T^{L} x_{st} \tag{4.65}$$

$$extra\_cw(u) = W(u)\, cp_{fluid} G_{cw} \tag{4.66}$$

$$extra\_st(u) = W(u)\, cp_{fluid} G_{st} \tag{4.67}$$

Constraints (4.66) and (4.67) still contain bilinear terms and are therefore linearised using the reformulation-linearisation technique discussed in Section 3.4 of Chapter 3 (Sherali & Alameddine, 1992; Quesada & Grossmann, 1995). Constraint (4.66) is linearised using Constraints (4.68) to (4.74) and Constraint (4.67) is linearised using Constraints (4.75) to (4.81). Constraints (4.82) and (4.83) are then obtained.

$$W(u) G_{cw} = K_{cw} \tag{4.68}$$

$$W^{L} \leq W(u) \leq W^{U} \tag{4.69}$$

$$\Delta T^{L} \leq G_{cw} \leq \Delta T^{U} \tag{4.70}$$

$$K_{cw} \leq W^{U} G_{cw} + \Delta T^{L} W(u) - W^{U} \Delta T^{L} \tag{4.71}$$

$$K_{cw} \leq W^{L} G_{cw} + \Delta T^{U} W(u) - W^{L} \Delta T^{U} \tag{4.72}$$

$$K_{cw} \geq W^{L} G_{cw} + \Delta T^{L} W(u) - W^{L} \Delta T^{L} \tag{4.73}$$

$$K_{cw} \geq W^{U} G_{cw} + \Delta T^{U} W(u) - W^{U} \Delta T^{U} \tag{4.74}$$

$$W(u) G_{st} = K_{st} \tag{4.75}$$

$$W^{L} \leq W(u) \leq W^{U} \tag{4.76}$$

$$\Delta T^{L} \leq G_{st} \leq \Delta T^{U} \tag{4.77}$$

$$K_{st} \leq W^{U} G_{st} + \Delta T^{L} W(u) - W^{U} \Delta T^{L} \tag{4.78}$$

$$K_{st} \leq W^{L} G_{st} + \Delta T^{U} W(u) - W^{L} \Delta T^{U} \tag{4.79}$$

$$K_{st} \geq W^{L} G_{st} + \Delta T^{L} W(u) - W^{L} \Delta T^{L} \tag{4.80}$$

$$K_{st} \geq W^{U} G_{st} + \Delta T^{U} W(u) - W^{U} \Delta T^{U} \tag{4.81}$$

$$extra\_cw(u) = cp_{fluid} K_{cw} \tag{4.82}$$

$$extra\_st(u) = cp_{fluid} K_{st} \tag{4.83}$$

Constraint (4.84) is also necessary, as either extra cooling or extra heating will be required for the heat storage vessel at the end of the cycle, or neither will be required.

$$x_{cw} + x_{st} \leq 1 \tag{4.84}$$

If neither extra heating nor extra cooling are required to bring the heat storage temperature back to its initial temperature, T_{start} will be equal to T_{end} and the values for *extra_cw*(u) and *extra_st*(u) will both be zero.

In order for the heat storage temperature to return to its starting temperature, the total energy into the heat storage vessel must be equal to the energy out of the heat storage vessel within the cycle. Constraint (4.85) is used to ensure this.

$$\sum_{s_{in,j_h}} \sum_{p} Q\left(s_{in,j_h}, u, p\right) + extra\_st(u) = \sum_{s_{in,j_c}} \sum_{p} Q\left(s_{in,j_c}, u, p\right) + extra\_cw(u) \tag{4.85}$$

The profit is given by Equation (4.86).

$$\begin{aligned} \text{profit} = & \sum_{s} CP\left(s^{p}\right) q_{s}\left(s^{p}, p\right) - Cost\_cw \sum_{s_{in,j_h}} \sum_{p} cw\left(s_{in,j_h}, p\right) - Cost\_cw * extra\_cw(u) \\ & - Cost\_st \sum_{s_{in,j_c}} \sum_{p} st\left(s_{in,j_c}, p\right) - Cost\_st * extra\_st(u), \\ & \forall p = P, \quad s_{in,j_h} \in S_{in,j}, \quad s_{in,j_c} \in S_{in,j}, \quad s^{p} \in S^{p} \end{aligned} \tag{4.86}$$

The objective for the cyclic period is then to maximise the average profit per cycle, as given by Constraint (4.87).

$$Max \frac{profit}{H} \tag{4.87}$$

The solution procedure discussed in Section 3.4 of Chapter 3 was also applied in this Chapter. Constraints (4.40) to (4.51), Constraints (4.54) to (4.65) and Constraints (4.68) to (4.87) are used in the linearised model, while Constraints (4.40) to (4.51), Constraints (4.54) to (4.67) and Constraints (4.84) to (4.87) are used in the exact model. This is in addition to the scheduling and heat integration constraints and applies to the determination of the optimal cyclic schedule.

Once the optimal cycle length has been determined, the initial and final periods can be solved. The overall objective is the maximisation of profit over the entire long time horizon.

4.5 Simple linear process

A simple linear scheduling problem was modified to include heat integration data to provide opportunities for heat integration (Seid & Majozi, 2012). Figure 4.4 shows the state task network, while Figure 4.5 shows the state sequence network for the process.

Figure 4.4. STN for simple process.

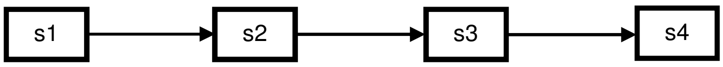

Figure 4.5. SSN for simple process.

The necessary scheduling data can be found in Table 4.1 and Table 4.2, while the heat integration parameters and heating and cooling requirements may be found in Table 4.3 and Table 4.4, respectively.

Table 4.1. Scheduling data for simple process.

Unit	Capacity	Suitability	Mean processing time (h)
Mixer	100	Mixing	4.5
Reactor	75	Reaction	3
Purificator	50	Purification	1.5

Table 4.2. Scheduling data for simple process.

State	Storage capacity (ton)	Initial amount (ton)	Revenue (c.u./ton)
s1	unlimited	unlimited	0
s2	100	0	0
s3	100	0	0
s4	unlimited	0	1

Table 4.3. Heat integration data for simple process.

Parameter	Value
Specific heat capacity, cp_{fluid} (kJ/kg°C)	4.2
Product selling price (c.u./ton)	1
Steam cost (c.u./kWh)	0.08
Cooling water cost (c.u./kWh)	0.02
$\Delta T^{\min}$ (°C)	10
T^L (°C)	20
T^U (°C)	180
ΔT^L (°C)	0
ΔT^U (°C)	180
W^L (ton)	0.1
W^U (ton)	2

Table 4.4. Heating/cooling requirements for simple process.

Task	Type	Max heating/cooling requirement (kWh)	Operating temperature (°C)
Reaction	exothermic	50 (cooling)	120
Purification	endothermic	40 (heating)	70

Cyclic portion

As the model used to solve the cyclic portion contains nonlinear terms, the same linearisation technique and solution procedure as used in Section 3.4 of Chapter 3 was used. The objective function will, however, still contain a nonlinearity which cannot be linearised and as such, both the linearised and exact models will be MINLP problems. The problem was solved with GAMS 24.1.3 using DICOPT for the MINLP with CPLEX as the MIP solver and MINOS5 as the NLP solver. All models were solved using a computer with an Intel Core i3, 3.1 GHz processor with 2.0 GB RAM.

The results obtained for the cyclic portion can be seen in Table 4.5. The optimal cycle length is 9 h and an average profit of 21.837 c.u./h is achieved. The CPU times are the sum of the CPU times for both the linearised and the exact models.

Table 4.5. Results of cyclic portion for simple process.

Cycle range (h)	Optimal cycle time (h)	Objective (c.u./h)	Time points	CPU time (s)
3 – 6	4.5	16.489	4	2.339
6 – 9	9	21.837	7	275.338
9 – 12	9	21.837	7	52.033

The results obtained for the optimal schedule for the optimal cycle length of 9 h are shown in Table 4.6.

Table 4.6. Results of optimal cyclic length for simple process.

Starting and ending amount of intermediate state (ton)		
	s2	100
	s3	0
Starting and ending storage temperature (°C)		80
Heat storage size (ton)		0.952
Cooling water (kWh)		13.333
Steam (kWh)		40
Extra cooling water (kWh)		0
Extra steam (kWh)		0

The optimal schedule obtained is shown in Figure 4.6.

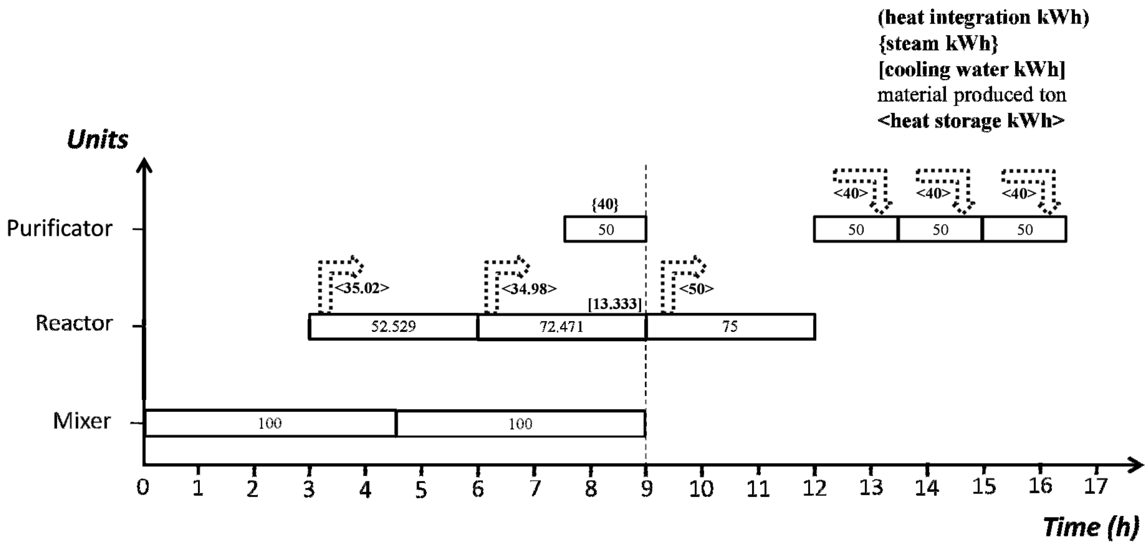

Figure 4.6. Gantt chart for optimal cycle length (9 h) for simple process.

Initial period

In order to solve for the initial period of the time horizon, the amounts of intermediates at the end of the initial period are fixed to the values required to start the cyclic period. These values are obtained from the solution of the cyclic scheduling portion. This is to ensure there will be sufficient of the intermediate states produced in the initial period to be available to start the cyclic scheduling period. First, a makespan minimisation problem is solved to determine a feasible time horizon for the initial period. A profit maximisation problem is then solved in order to maximise the profit in the initial period. The optimum heat storage size of 0.952 ton which was solved for in the cyclic period is now fixed in the initial period. Since this is the case, both the makespan minimisation and profit maximisation problems will be MILP problems. The heat storage vessel was not utilised during the initial period and the heat storage temperature therefore remains at 80℃.

From the makespan minimisation problem, a feasible time horizon of 4.5 h was determined for the initial period, in a CPU time of 0.078 s and required 2 time points. The Gantt chart for the profit maximisation problem over 4.5 h is shown in Figure 4.7 and the results are shown in Table 4.7.

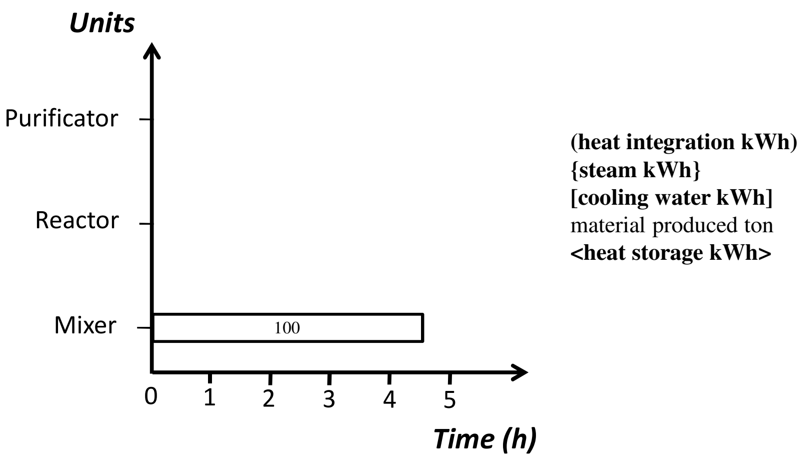

Figure 4.7. Gantt chart for maximisation of profit over initial period (4.5 h) for simple process.

Table 4.7. Results for maximisation of profit over initial period for simple process.

Time period (h)	4.5
Objective (c.u.)	0
Time points	2
Cooling water (kWh)	0
Steam (kWh)	0
CPU time (s)	0.062

Final period

A total time horizon of 24 h was chosen. Repeating the cyclic portion once and accounting for the initial period of 4.5 h, a final period of 10.5 h remains. A profit maximisation problem was solved for the final period and an objective value of 150 c.u. was determined in a CPU time of 0.156 s and required 5 time points.

The Gantt chart for the profit maximisation over the final period is shown in Figure 4.8 and the results are shown in Table 4.8.

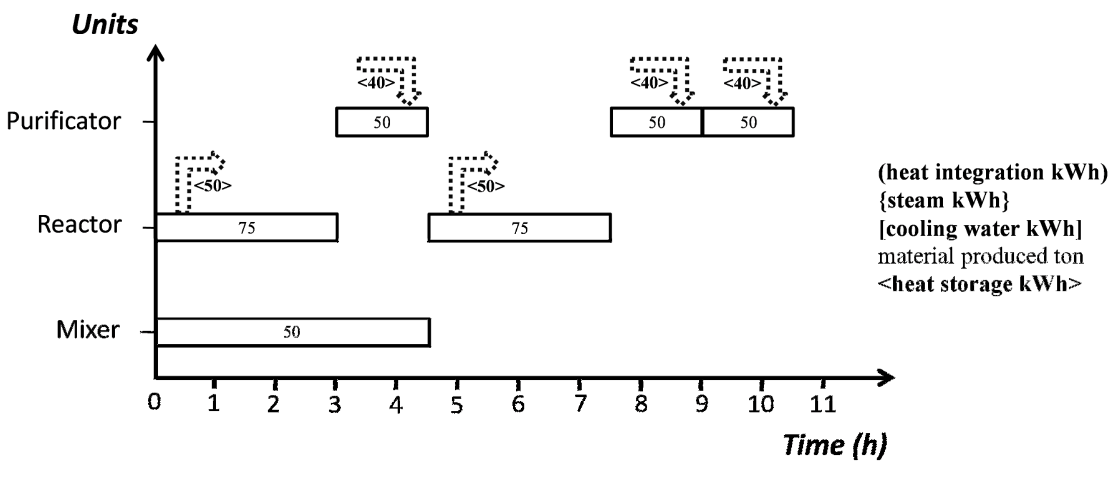

Figure 4.8. Gantt chart for maximisation of profit over final period (10.5 h).

Table 4.8. Results of profit maximisation over final period for simple process.

Time period (h)	10.5
Objective (c.u.)	150
Time points	5
Cooling water (kWh)	0
Steam (kWh)	0
CPU time (s)	0.156

Comparison with direct solution

The heat integration problem was solved directly over a time horizon of 24 h. The same 2-step solution procedure of Section 3.4 of Chapter 3 was used, as the model contains nonlinear terms. The direct solution gives a profit of 348.667 c.u. This solution was compared to the solution achieved using the cyclic scheduling heat integration model. For the cyclic scheduling model, the profit from each period (initial, cyclic and final) is added to give a total profit over the long time horizon. The profit for the cyclic period is obtained by multiplying the average profit over the cycle (21.837 c.u./h) by the cycle time (9 h) and the number of times the cycle is repeated (once), which gives 196.533 c.u. In this case, the total profit is 346.533 c.u. (0 c.u. + 196.533 c.u. + 150 c.u.). The profit from the exact solution was 0.612% better than the profit obtained using the cyclic scheduling method.

The problem was also solved directly for the case where only direct heat integration was used as well as the case where only utilities were available for heating and cooling. The results for the exact solutions for all three cases are shown in Table 4.9.

Table 4.9. Results of direct solution of simple problem for three cases over 24 h.

	Utilities only	Direct heat integration	Heat storage
Objective (c.u.)	322.933	334.120	348.667
Cooling water (kWh)	233.333	134.804	66.667
Steam (kWh)	280	164.804	0
Time points	9	10	12
CPU time (s)	0.08	1.82	1 538
Initial storage temperature (°C)			96.5
Heat storage size (ton)			1.058

From Table 4.9, the objective value increases when direct heat integration is applied compared to the utilities only case and increases even further with the inclusion of heat storage.

The cyclic scheduling model was also solved for the cases of direct heat integration only and the utilities only case. The comparisons between the exact solutions and the cyclic scheduling solutions for all three cases are shown in Table 4.10.

Table 4.10. Comparison between direct solution and cyclic scheduling solution over 24 h.

Period	Duration (h)	Profit (c.u.)	Direct solution (c.u.)	% Error from exact solution
Heat integration with storage				
Initial	4.5	0		
Cyclic	9	196.533		
Final	10.5	150		
Overall	24	346.533	348.667	0.612
Direct heat integration				
Period	Duration (h)	Profit (c.u.)	Direct solution (c.u.)	% Error from exact solution
Initial	9	22.4		
Cyclic	9	191.2		
Final	6	119.0		
Overall	24	332.6	334.12	0.455
Utilities only				
Period	Duration (h)	Profit (c.u.)	Direct solution (c.u.)	% Error from exact solution
Initial	4.5	0		
Cyclic	9	184.533		
Final	10.5	138.4		
Overall	24	322.933	322.933	0.0

4.6 Multipurpose example

Figure 4.9 shows the state task network of a multipurpose batch plant, while Figure 4.10 shows the state sequence network (Seid & Majozi, 2012). This example is commonly referred to as “BATCH1” in literature and has been modified to include heating and cooling for certain tasks to allow for the possibility of heat integration. For this example, the batch sizes were not fixed and the energy requirements varied linearly with batch size.

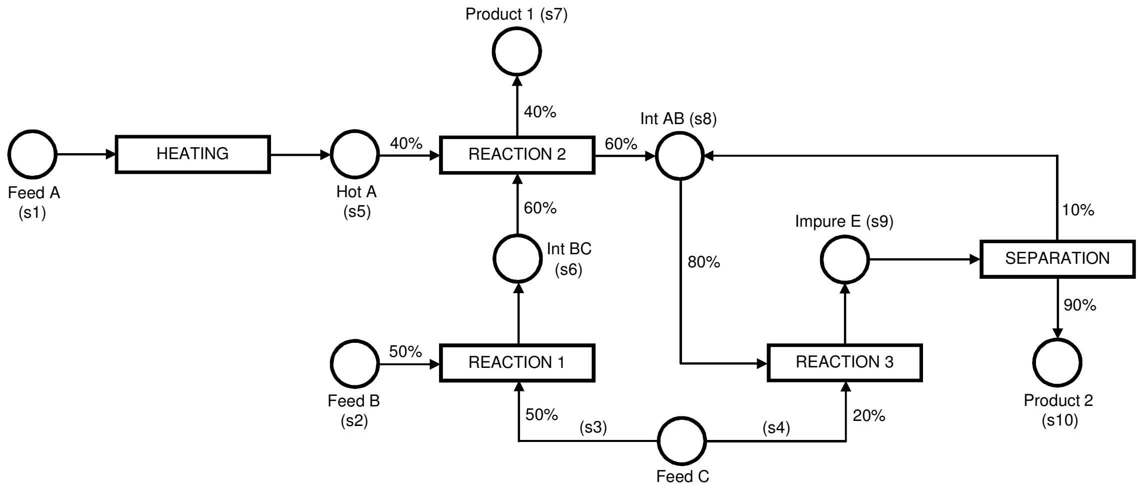

Figure 4.9. STN for multipurpose example.

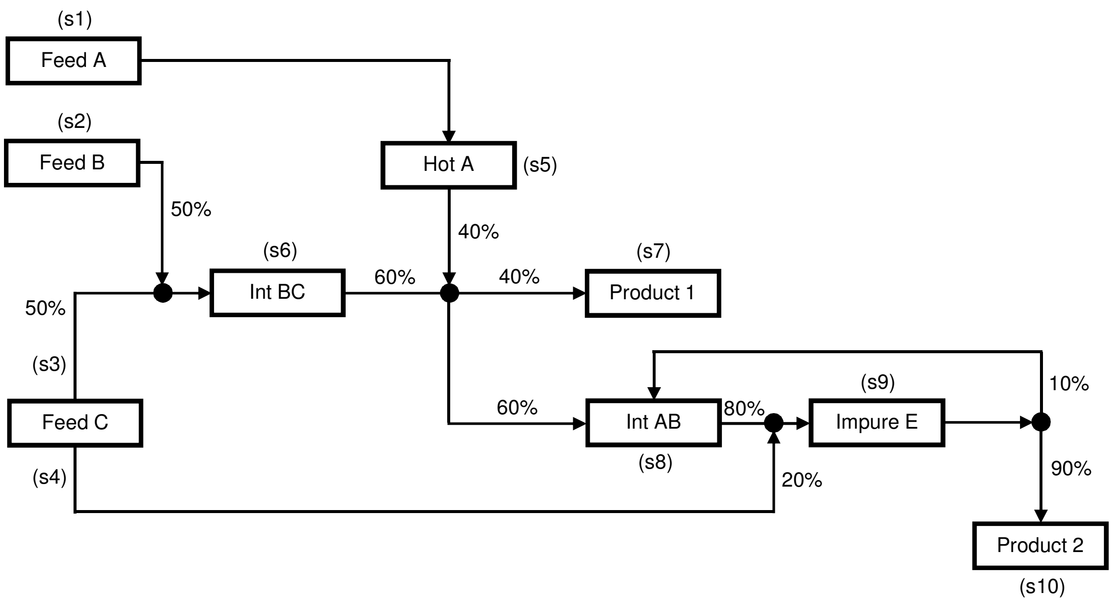

Figure 4.10. SSN for multipurpose example.

The required scheduling data may be found in Table 4.11 and Table 4.12, while the necessary heat integration data and heating and cooling requirements may be found in Table 4.13 and Table 4.14, respectively.

Table 4.11. Scheduling data for multipurpose example.

Unit	Capacity	Suitability	Mean processing time (h)
Heater	100	Heating	1
Reactor 1	50	RX1, RX2, RX3	2, 2, 1
Reactor 2	80	RX1, RX2, RX3	2, 2, 1
Still	200	Separation	1 (Product 2) 2 (Int AB)

Table 4.12. Scheduling data for multipurpose example.

State	Storage capacity (ton)	Initial amount (ton)	Revenue (c.u./ton)
Feed A (s1)	unlimited	unlimited	0
Feed B (s2)	unlimited	unlimited	0
Feed C (s3/s4)	unlimited	unlimited	0
Hot A (s5)	100	0	0
Int AB (s8)	200	0	0
Int BC (s6)	150	0	0
Impure E (s9)	200	0	0
Product 1	unlimited	0	100
Product 2	unlimited	0	100

Table 4.13. Heat integration data for multipurpose example.

Parameter	Value
Specific heat capacity, cp_{fluid} (kJ/kg°C)	4.2
Product selling price (c.u./ton)	100
Steam cost (c.u./kWh)	10
Cooling water cost (c.u./kWh)	2
$\Delta T^{\min}$ (°C)	10
T^L (°C)	20
T^U (°C)	250
ΔT^L (°C)	0
ΔT^U (°C)	250
W^L (ton)	0.1
W^U (ton)	4

Table 4.14. Heating/cooling requirements for multipurpose example.

Task	Type	Max heating/cooling requirement (kWh)	Operating temperature (ºC)
RX1	exothermic	60 (cooling)	100
RX2	endothermic	80 (heating)	60
RX3	exothermic	70 (cooling)	140

Cyclic portion

The results obtained for the cyclic portion can be seen in Table 4.15. The optimal cycle length is 5 h and an average profit of 3 581.920 c.u./h is achieved. The CPU times in the table are the sum of the CPU times for both the linearised and the exact models.

Table 4.15. Results of cyclic portion for multipurpose example.

Cycle range (h)	Optimal cycle time (h)	Objective (c.u./h)	Time points	CPU time (s)
3 – 6	5	3 581.920	6	204.55
6 – 9	6	3 478.086	7	1 781.50
9 – 12	12	3 560.000	9	280 048.74

The results obtained for the optimal schedule for the optimal cycle length of 5 h are shown in Table 4.16. The optimal schedule obtained is shown in Figure 4.11.

Table 4.16. Results of optimal cyclic length for multipurpose example.

Starting and ending amount of intermediate state (ton)		
	s5	0
	s6	0
	s8	48
	s9	150
Starting and ending storage temperature (°C)		70
Heat storage size (ton)		0.357
Cooling water (kWh)		95.2
Steam (kWh)		0
Extra cooling water (kWh)		0
Extra steam (kWh)		0

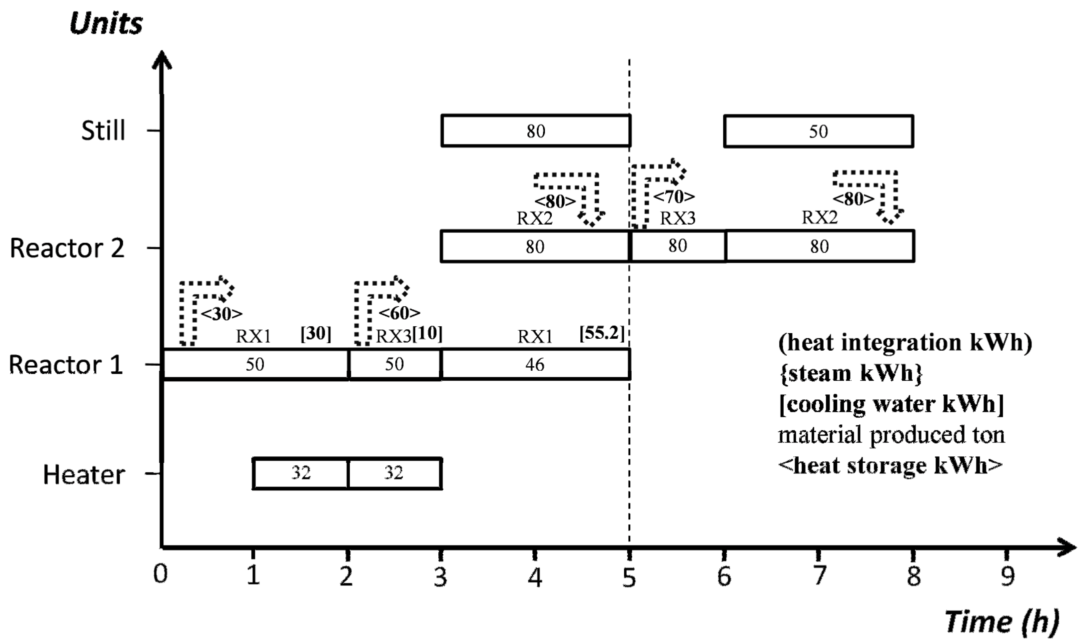

Figure 4.11. Gantt chart for optimal cycle length (5 h) for multipurpose example.

Initial period

The amounts of intermediate states at the end of the initial period are fixed to the values required to start the cyclic period to ensure there will be sufficient of the intermediate states produced in the initial period available to start the cyclic scheduling period. The optimum heat storage size of 0.357 ton which was solved for in the cyclic portion is now fixed in the initial period. The final temperature for the heat storage vessel is set at 70°C.

From the makespan minimisation problem, a feasible time horizon of 9 h was determined for the initial period, in a CPU time of 0.593 s and required 6 time points. The Gantt chart for the profit maximisation problem over 9 h is shown in Figure 4.12 and the results are shown in Table 4.17.

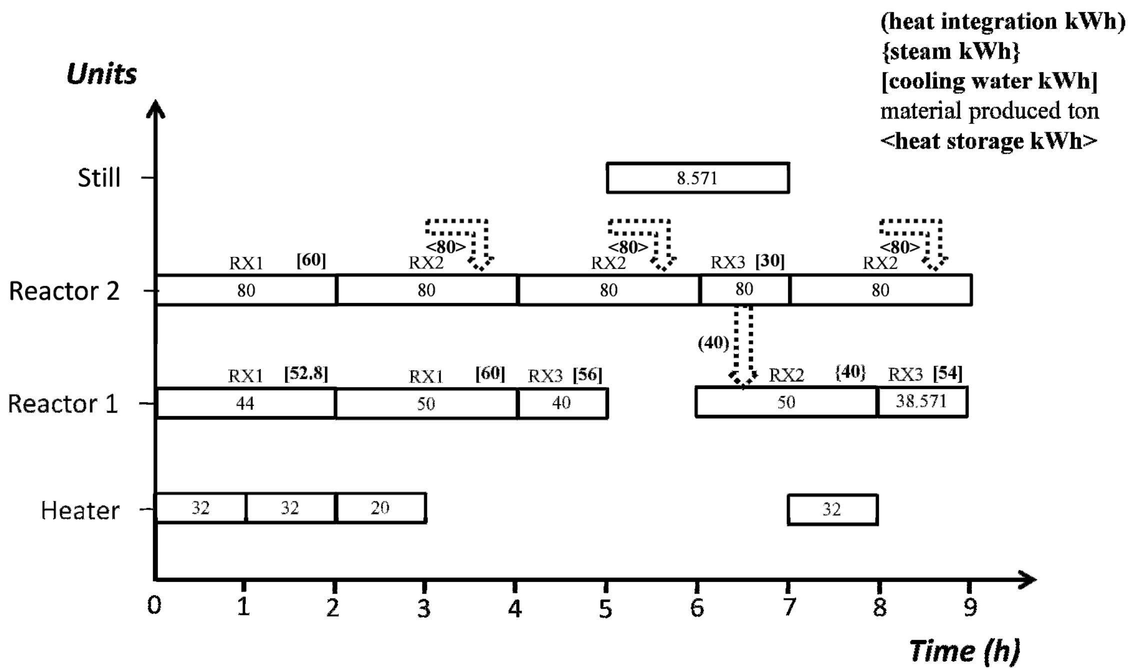

Figure 4.12. Gantt chart for maximisation of profit over initial period (9 h) for multipurpose example.

Table 4.17. Results for maximisation of profit over initial period for multipurpose example.

Time period (h)	9
Objective (c.u.)	11 345.829
Time points	6
Cooling water (kWh)	321.8
Steam (kWh)	40
Initial heat storage temperature (°C)	230.064
CPU time (s)	0.983

Final period

A total time horizon of 24 h was chosen. Repeating the cyclic portion once and accounting for the initial period of 9 h, a final period of 10 h remains. A profit maximisation problem was solved for the final period and an objective value of 46 605.928 c.u. was determined in a CPU time of 1.794 s and required 6 time points.

The Gantt chart for the maximisation of profit over the final period is shown in Figure 4.13 and the results are shown in Table 4.18.

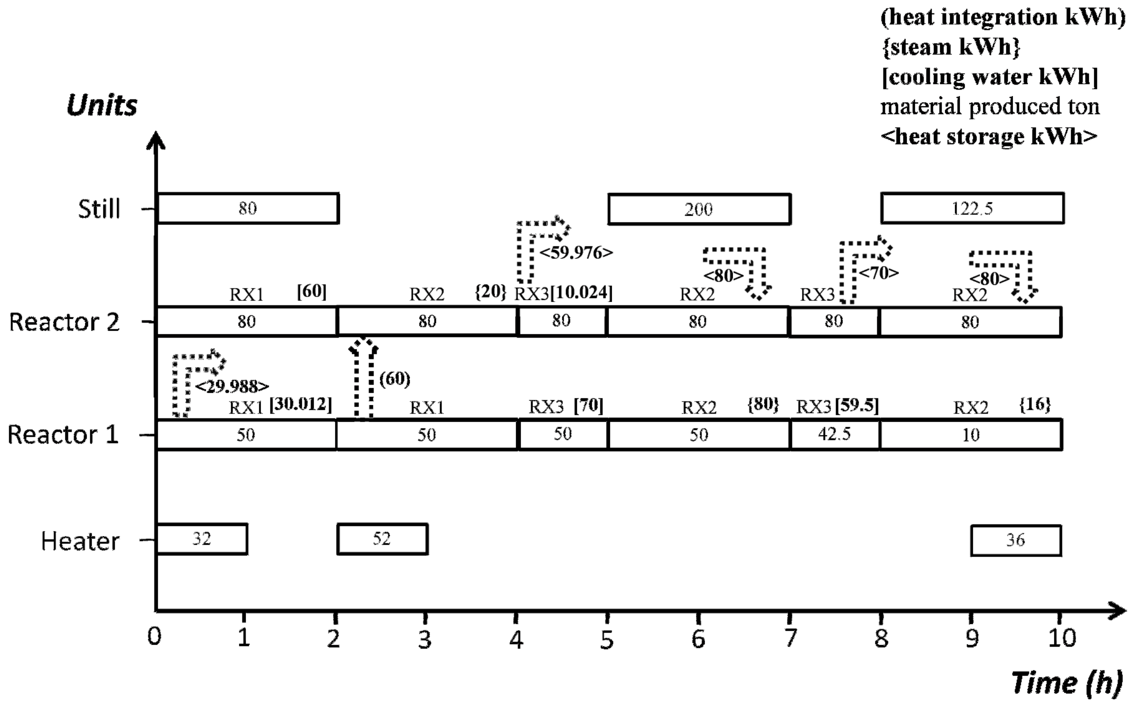

Figure 4.13. Gantt chart for maximisation of profit over final period (10 h) for multipurpose example.

Table 4.18. Results for maximisation of profit over final period for multipurpose example.

Time period (h)	10
Objective (c.u.)	46 605.928
Time points	6
Cooling water (kWh)	229.54
Steam (kWh)	116
CPU time (s)	1.794

Comparison with direct solution

The problem was also solved for the case where only direct heat integration was used as well as the case where only utilities were available for heating and cooling. In order to have a long enough time horizon for a fair comparison, the problem becomes too complex to solve directly for the heat storage case. A fairly long final period is required as most of the products are formed during this time and this makes the overall time horizon lengthy. However, the results for the direct solution of the problem for the other two cases are shown in Table 4.19 as well as a summary of the results for the cyclic scheduling heat integration model. The objective value of 76 580 c.u. for the direct solution for the case where only direct heat integration was used was determined in a CPU time of 1 106.922 s and required 16 time points. The objective value of 70 790 c.u. for the direct solution for the case where only external utilities were available was determined in a CPU time of 1 405.156 s and required 16 time points.

Table 4.19. Comparison between direct solution and cyclic scheduling solution over 24 h.

Period	Duration (h)	Profit (c.u.)	Direct solution (c.u.)	% Error from exact solution
Heat integration with storage				
Initial	9	11 345.8		
Cyclic	5	17 909.6		
Final	10	46 605.9		
Overall	24	75 861.4	-	-
Direct heat integration				
Period	Duration (h)	Profit (c.u.)	Direct solution (c.u.)	% Error from exact solution
Initial	6	5 547.2		
Cyclic	5 (x2)	34 744.0		
Final	8	31 840.0		
Overall	24	72 131.2	76 580	5.809
Utilities only				
Period	Duration (h)	Profit (c.u.)	Direct solution (c.u.)	% Error from exact solution
Initial	11	10 312.8		
Cyclic	5	15 989.6		
Final	8	40 840.0		
Overall	24	67 142.4	70 790	5.153

4.7 Industrial case study

Figure 4.14 shows the state task network of an industrial case study, while Figure 4.15 shows the state sequence network (Chen & Chang, 2009).

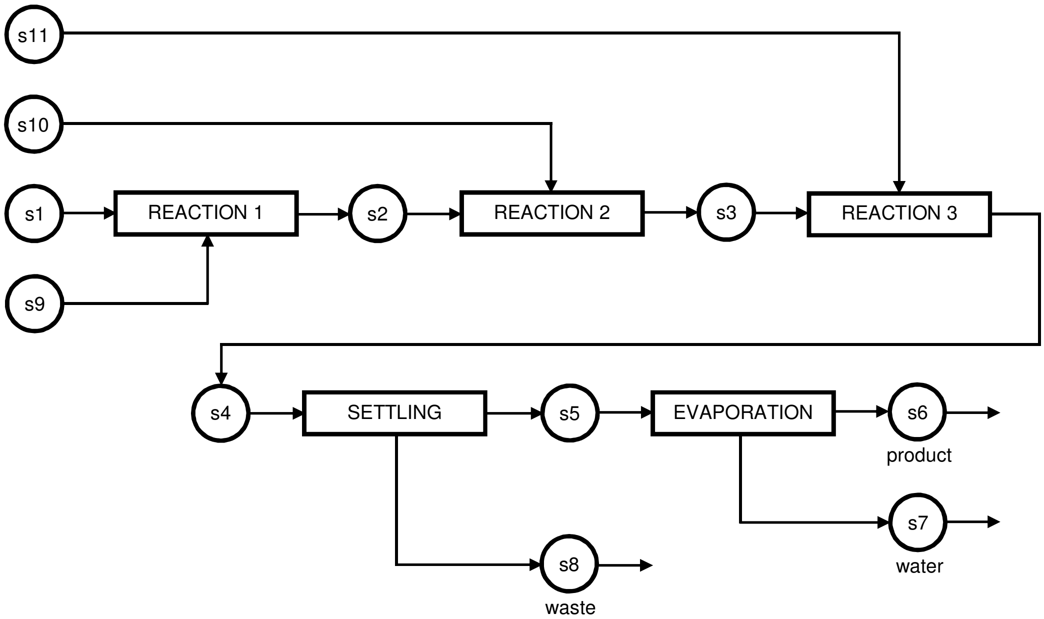

Figure 4.14. STN for industrial case study.

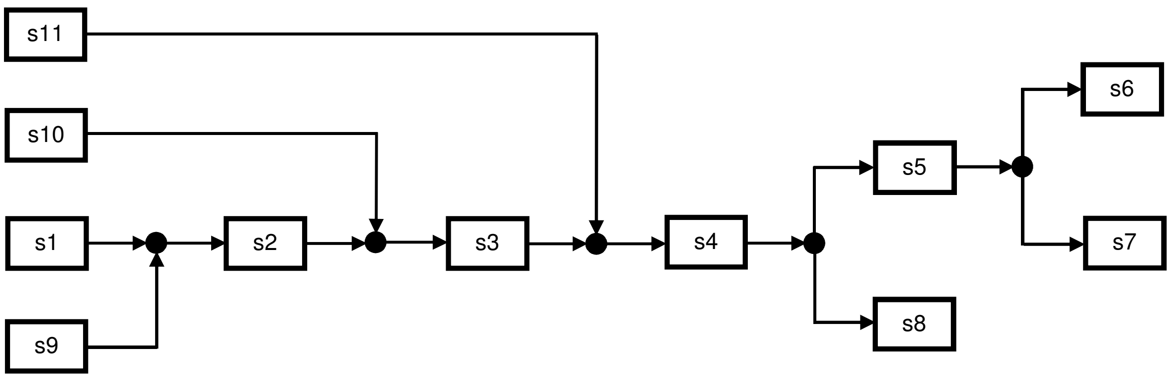

Figure 4.15. SSN for industrial case study.

The scheduling data for the problem may be found in Table 4.20 and Table 4.21 with the stoichiometric data available in Table 4.22. The heat integration data and heating and cooling requirements may be found in Table 4.23 and Table 4.24, respectively.

Table 4.20. Scheduling data for industrial case study.

Unit	Capacity	Suitability	Mean processing time (h)
R1	10	RX1	2
R2	10	RX1	2
R3	10	RX2, RX3	3, 1
R4	10	RX2, RX3	3, 1
SE1	10	Settling	1
SE2	10	Settling	1
SE3	10	Settling	1
EV1	10	Evaporation	3
EV2	10	Evaporation	3

Table 4.21. Scheduling data for industrial case study.

State	Storage capacity (ton)	Initial amount (ton)	Revenue (c.u./ton)
s1	unlimited	unlimited	0
s2	100	0	0
s3	100	0	0
s4	100	0	0
s5	100	0	0
s6	100	0	10 000
s7	100	0	0
s8	100	0	0
s9	unlimited	unlimited	0
s10	unlimited	unlimited	0
s11	unlimited	unlimited	0

Table 4.22. Stoichiometric data for industrial case study.

State	Ton/ton output	Ton/ton product
s1	0.20	
s9	0.25	
s10	0.35	
s11	0.20	
s7		0.7
s8		1

Table 4.23. Heat integration data for industrial case study.

Parameter	Value
Specific heat capacity, cp_{fluid} (kJ/kg°C)	4.2
Product selling price (c.u./ton)	10 000
Steam cost (c.u./kWh)	20
Cooling water cost (c.u./kWh)	8
$\Delta T^{\min}$ (°C)	5
T^{L} (°C)	20
T^{U} (°C)	180
ΔT^{L} (°C)	0
ΔT^{U} (°C)	180
W^{L} (ton)	0.1
W^{U} (ton)	1.5

Table 4.24. Heating/cooling requirements for industrial case study.

Task	Type	Max heating/cooling requirement (kWh)	Operating temperature (°C)
RX2	exothermic	100 (cooling)	150
Evaporation	endothermic	110 (heating)	90

Cyclic portion

The results obtained for the cyclic portion can be seen in Table 4.25. The optimal cycle length is 9 h and an average profit of 20 528.395 c.u./h is achieved. The CPU times in the table are the sum of the CPU times for both the linearised and the exact models.

Table 4.25. Results of cyclic portion for industrial case study.

Cycle range (h)	Optimal cycle time (h)	Objective (c.u./h)	Time points	CPU time (s)
3 – 6	4	18 475.556	3	1.079
6 – 9	9	20 528.395	6	123.734
9 – 12	9	20 528.395	6	42.137

The results obtained for the optimal schedule for the optimal cycle length of 9 h are shown in Table 4.26. The optimal schedule obtained is shown in Figure 4.16.

Table 4.26. Results of optimal cyclic length for industrial case study.

Starting and ending amount of intermediate state (ton)		
	s2	5.625
	s3	30
	s4	10
	s5	4.882
Starting and ending storage temperature (°C)		95
Heat storage size (ton)		0.22
Cooling water (kWh)		53.704
Steam (kWh)		0
Extra cooling water (kWh)		0
Extra steam (kWh)		0

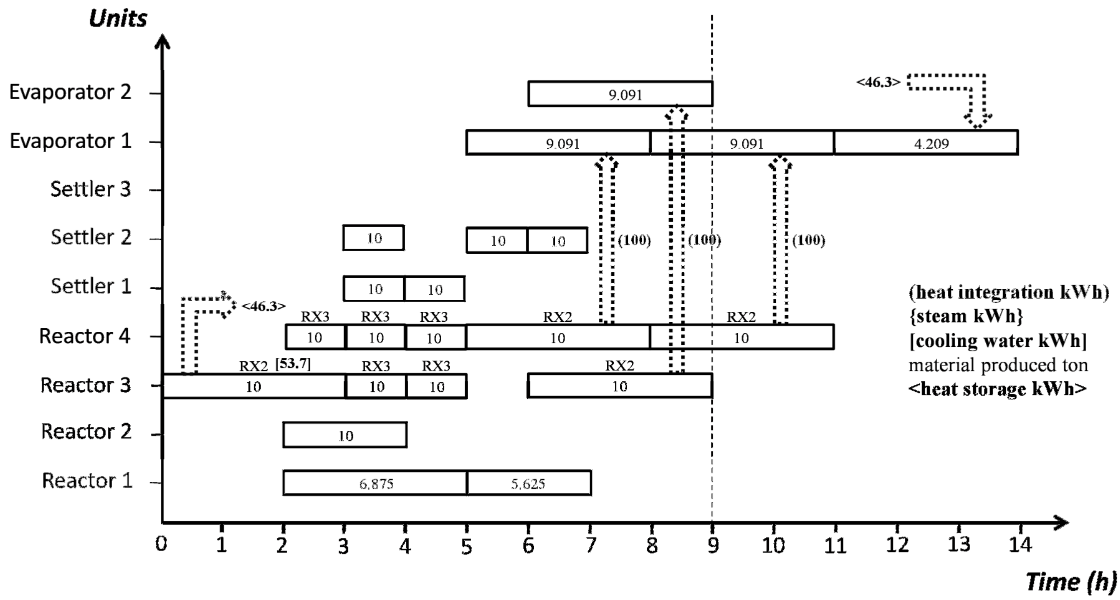

Figure 4.16. Gantt chart for optimal cycle length (9 h) for industrial case study.

Initial period

The amounts of intermediate states at the end of the initial period are fixed to the values required to start the cyclic period to ensure there will be sufficient of the intermediate states produced in the initial period available to start the cyclic scheduling period. The optimum heat storage size of 0.22 ton, which was solved for in the cyclic period, is now fixed in the initial period. The final temperature for the heat storage vessel is set at 95°C.

From the makespan minimisation problem, a feasible time horizon of 11 h was determined for the initial period, in a CPU time of 0.73 s and required 6 time points. The Gantt chart for the profit maximisation problem over 11 h is shown in Figure 4.17 and the results are shown in Table 4.27.

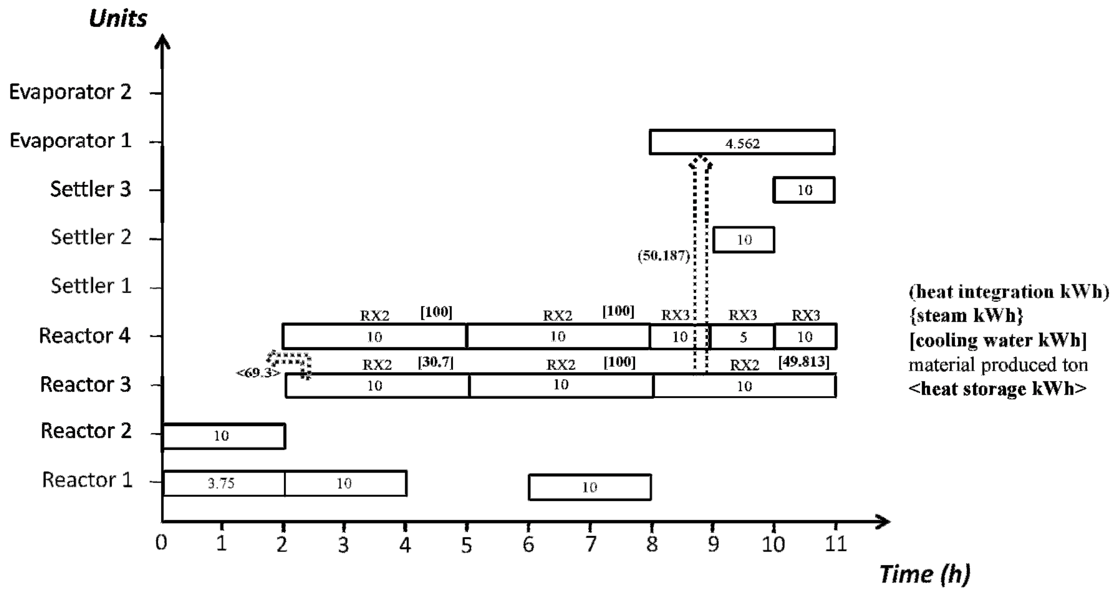

Figure 4.17. Gantt chart for maximisation of profit over initial period (11 h) for industrial case study.

Table 4.27. Results for maximisation of profit over initial period for industrial case study.

Time period (h)	11
Objective (c.u.)	23 793.804
Time points	7
Cooling water (kWh)	380.513
Steam (kWh)	0
Initial heat storage temperature (°C)	20
CPU time (s)	81.89

Final period

A total time horizon of 48 h was chosen. Repeating the cyclic portion three times and accounting for the initial period of 11 h, a final period of 10 h remains. A profit maximisation problem was solved for the final period and an objective value of 338 884.348 c.u. was determined in a CPU time of 1 515.2 s and required 9 time points.

The Gantt chart for the profit maximisation over the final period is shown in Figure 4.18 and the results are shown in Table 4.28.

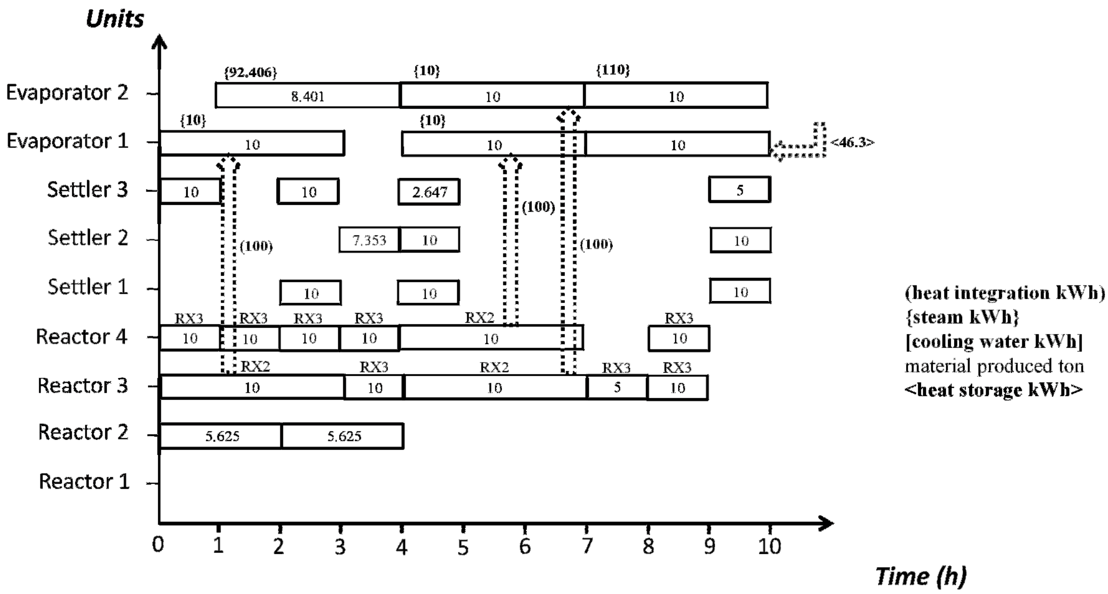

Figure 4.18. Gantt chart for maximisation of profit over final period (10 h) for industrial case study.

Table 4.28. Results for maximisation of profit over final period for industrial case study.

Time period (h)	10
Objective (c.u.)	338 884.348
Time points	9
Cooling water (kWh)	0
Steam (kWh)	232.406
CPU time (s)	1 515.2

The problem was also solved for the case with direct heat integration only as well as the case where only utilities are available. A summary of results for each case is given in Table 4.29. In each case, the cyclic period was repeated three times.

Table 4.29. Results of cyclic scheduling for different cases over 48 h for industrial case study.

Heat integration with storage		
Period	Duration (h)	Profit (c.u.)
Initial	11	23 793.804
Cyclic	9 (x3)	554 266.665
Final	10	338 884.348
Overall	48	916 944.817
Direct heat integration		
Period	Duration (h)	Profit (c.u.)
Initial	13	11 625.325
Cyclic	9 (x3)	554 266.668
Final	8	234 494.118
Overall	48	800 386.111
Utilities only		
Period	Duration (h)	Profit (c.u.)
Initial	14	6 457.583
Cyclic	9 (x3)	525 177.777
Final	7	226 494.118
Overall	48	758 129.478

Comparison with existing literature model

This same example was considered by Chen and Chang (2009). In solving for the optimal cycle length, a series of fixed values were used and the cycle time giving the best objective, which is the average profit per time, was considered optimal. The model proposed in this chapter, however, includes the optimal cycle length as an optimisation variable which is solved for between a given upper and lower bound. Also, the initial and final periods of the time horizon were not considered in the model of Chen and Chang (2009).

To compare the models, the heat integration and cost data as used by Chen and Chang (2009) were used. These values may be obtained from Table 4.30. In the example, batch sizes were not fixed and the maximum batch sizes were given as 8 ton for all units. Only direct heat integration was considered.

Table 4.30. Data for comparison of industrial case study.

Product	Selling price ($/ton)
s6	100
Utility	**Unit cost ($/ton)**
Cooling water	8
Steam	15
Task	**Cooling/ Heating duty (ton)**
Reaction 2	5
Evaporation	4

The model proposed in this chapter, with direct heat integration only, was used to solve for the optimal cycle time between 6 h and 9 h and the same optimal objective value of $161.05 was obtained. The proposed model was also applied over an interval of 9 h to 12 h. The optimal cycle time was found to be 11 h and gave a better objective value of $164.71 compared to $161.05 for the reported optimal cycle time of 9 h.

4.8 Conclusions

A model for the cyclic scheduling of multipurpose batch plants using direct and indirect heat integration has been presented. Cyclic scheduling constraints were incorporated into the heat integration model of Stamp and Majozi (2011). The presented cyclic scheduling model can be used for any chosen long time horizon. Once the cyclic and initial portions have been solved, the flexibility of the model allows the solution over any long time horizon, as only the profit maximisation problem of the final period must be solved for again. Therefore, the time horizon does not affect the computational complexity required to solve the model.

The model may give better results when compared to an existing method as the cycle time is an optimisation variable rather than a fixed value and both the initial and final periods are also accounted for.

The model may be preferred for the solution of problems over long time horizons as direct solution using short-term methods may not be feasible. The direct solution for a simple sequential process over 24 h was compared to the solution obtained using the proposed cyclic heat integration model with heat storage and was better by only 0.612%.

4.9 References

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CHAPTER 5

CONCLUSIONS AND RECOMMENDATIONS

An overview of the relevant literature pertaining to this thesis regarding short-term scheduling, long-term scheduling and heat integration in batch plants was presented. A brief discussion on wastewater minimisation was also included.

A simultaneous method for the optimisation of energy and water embedded within a flexible scheduling framework was presented. Furthermore, opportunities for direct and indirect heat integration as well as direct and indirect water reuse were explored. The mathematical formulation led to a MINLP problem for which an initialisation procedure was employed.

The developed formulation proved effective in solving a complex makespan minimisation problem in which duration was a function of batch size and which included multiple contaminants. When compared to a published sequential method, an improved profit of 6.78% was achieved.

The model is such that it can easily be built upon and in order to increase the opportunities for water reuse, it is recommended that a regenerator be included for future work. The model can also be extended for solving fixed flow problems. Furthermore, the model can be applied to specific industries such as a brewery, which is both energy and water intensive.

A model for the cyclic scheduling of multipurpose batch plants using direct and indirect heat integration was presented. The model can be used for any chosen long time horizon. Once the cyclic and initial portions have been solved, the flexibility of the model allows the solution of any long time horizon, as only the profit maximisation problem of the final period must be solved for again. Therefore, the time horizon does not affect the computational complexity required to solve the model.

The model may give better results when compared to an existing method as the cycle time is an optimisation variable rather than a fixed value and both the initial and final periods are also accounted for.

The model may be preferred for the solution of problems over long time horizons as direct solution using short-term methods may not be feasible. The direct solution for a simple sequential process over 24 h was compared to the solution obtained using the proposed cyclic heat integration model with heat storage and was better by only 0.612%.

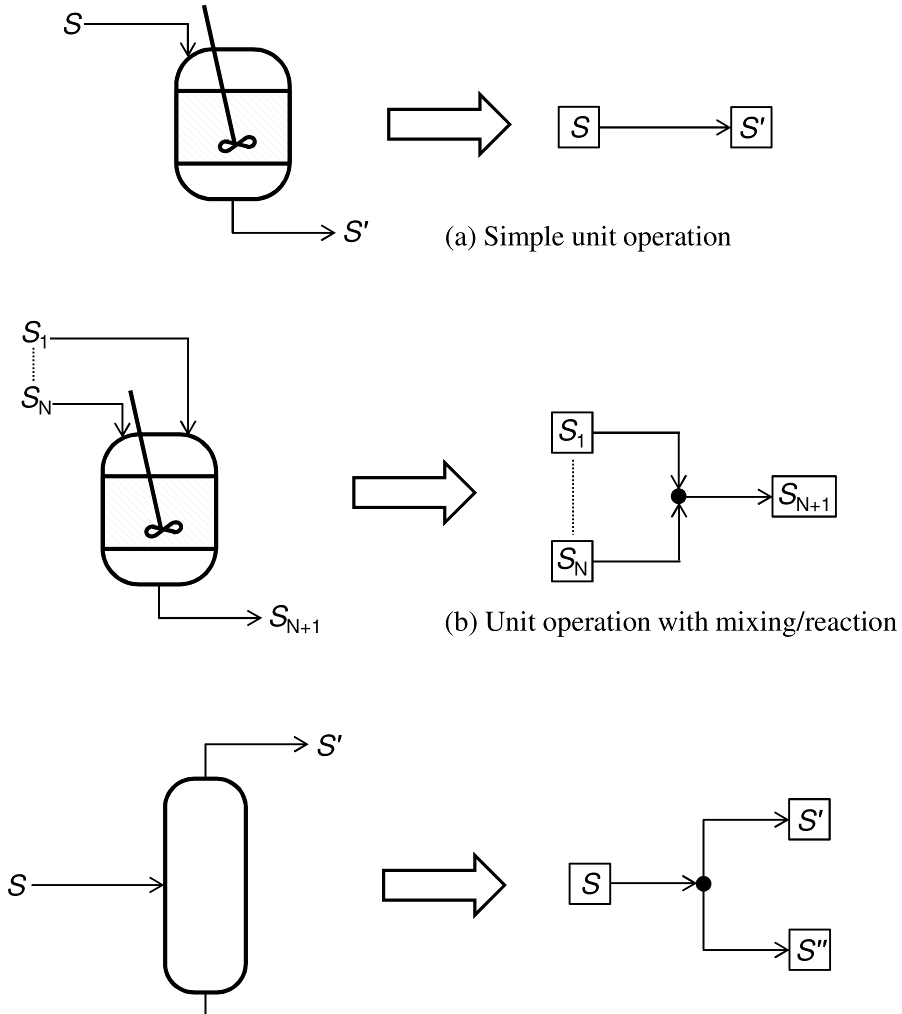
As it is becoming increasingly important to consider energy and water usage together rather than separately, it is recommended for future work that wastewater minimisation constraints be incorporated into the developed cyclic scheduling framework in order to make a comparison with the results obtained in Chapter 3 of this thesis.

APPENDICES

Appendix A: Scheduling model of Majozi and Zhu (2001)

The scheduling framework uses the state sequence network (SSN) recipe representation and an uneven discretisation of the time horizon. It is a unit specific event based formulation, where the time associated with events can be different across the units. This scheduling framework has proven to result in fewer binary variables compared to models based on other representations. The SSN representation is based on states only. Tasks and units are implicitly incorporated and this reduces the number of binary variables required for the solution. The only binary variable involved is $y(s_{in,j}, p)$, which equals one if state s is used in unit j at time point p and is zero otherwise. If more than one state enters a unit, only one input state needs to be defined as an effective state, as the other states will be inferred and $s_{in,j} \in S^*_{in,j}$, where $S^*_{in,j}$ is the set of effective states. The resulting model is a mixed integer linear programming (MILP) formulation. The building blocks of the SSN are shown in Figure A.1.

Figure A.1(a) shows the transition from state s to state s'. For example, this could be a washing operation with s as washing water and s' as effluent. This implies that there has to be a unit operation between these two due to the change in states. Figure A.1(b) shows the mixing of different states to yield a new state, e.g. raw materials entering a reactor to yield a product. Figure A.1(c) illustrates a splitting/separation unit with state s as the input and states s' and s'' as outputs.



(a) Simple unit operation

(b) Unit operation with mixing/reaction

(c) Unit operation with splitting

Figure A.1. Building blocks of state sequence network (SSN).

Capacity constraint

Constraint (A.1) states that the total amount of all the states consumed at time point p is limited by the capacity of the unit which consumes the states.

$$V_j^L y(s_{in,j}, p) \le \sum_{s_{in,j}} m_u(s,p) \le V_j^U y(s_{in,j}, p), \qquad \forall p \in P, \quad j \in J \qquad \text{(A.1)}$$

Material balances

Constraint (A.2) is the material balance around a particular unit *j*. It implies that the sum of the masses for all the input states used at time point *p*-1 should be equal to the sum of the masses for all the output states produced at time point *p*.

$$\sum_{s=s_{in,j}} m_u(s, p-1) = \sum_{s=s_{out,j}} m_p(s, p), \qquad \forall p \in P, p > p1, \quad j \in J \tag{A.2}$$

Constraint (A.3) states that the amount of state *s* stored at the first time point, is the difference between the amount stored before the beginning of the process and that being utilised at the first time point.

$$q_s(s, p1) = Q_s^0(s) - m_u(s_{in,j}, p1), \qquad \forall s_{in,j} \in S_{in,j}, \quad s \neq product \tag{A.3}$$

Constraint (A.4) is the storage balance applicable to feed states, as they are only used in the process.

$$q_s(s, p) = q_s(s, p-1) - m_u(s_{in,j}, p),$$
$$\forall p \in P, p > p1, \quad s_{in,j} \in S_{in,j}, \quad s = feed \tag{A.4}$$

Constraint (A.5) only applies to intermediates, since they are both produced and used in the process.

$$q_s(s, p) = q_s(s, p-1) + m_p(s_{out,j}, p) - m_u(s_{in,j}, p),$$
$$\forall p \in P, p > p1, \quad s_{in,j} \in S_{in,j}, \quad s_{out,j} \in S_{out,j}, \quad s \neq feed, product \tag{A.5}$$

Constraints (A.6) and (A.7) only apply to products and byproducts, since they are the only states that have to be taken out of the process as shown by the terms $d(s, p)$. Constraint (A.6) is used at the first time point and Constraint (A.7) is used for the remainder of the time horizon.

$$q_s(s, p1) = Q_s^0(s) - d(s, p1), \qquad s = product \tag{A.6}$$

$$q_s(s, p) = q_s(s, p-1) + m_p(s_{out,j}, p) - d(s, p),$$
$$\forall p \in P, p > p1, \quad s_{out,j} \in S_{out,j}, \quad s = product, byproduct \tag{A.7}$$

Duration constraints

Constraint (A.8) shows the duration of a task as a function of the batch size, while Constraint (A.9) is for a fixed task duration.

$$t_{out}(s_{out,j}, p) = t_u(s_{in,j}, p-1) + \alpha(s_{in,j})y(s_{in,j}, p-1) + \beta(s_{in,j})\sum_{s_{in,j}} mu(s, p-1),$$
$$\forall p \in P, p > p1, \quad s_{in,j} \in S_{in,j}, \quad s_{out,j} \in S_{out,j}, \quad j \in J \tag{A.8}$$

$$t_{out}(s_{out,j}, p) = t_u(s_{in,j}, p-1) + \tau(s_{in,j})y(s_{in,j}, p-1),$$
$$\forall p \in P, p > p1, \quad s_{in,j} \in S_{in,j}, \quad s_{out,j} \in S_{out,j}, \quad j \in J \tag{A.9}$$

Sequence constraints

Constraints (A.10) and (A.11) imply that state s can only be used in a particular unit, at any time point, after all the previous states have been processed. Constraint (A.10) is only relevant in situations where more than one task can be conducted in one unit, otherwise it is redundant in the presence of constraints (A.11) and (A.12).

$$t_u\left(s_{in,j},p\right) \geq \sum_{s_{in,j}} \sum_{s_{out,j}} \sum_{p' \leq p} t_{out}\left(s_{out,j},p'\right) - t_u\left(s_{in,j},p'-1\right),$$
$$\forall p, p' \in P,\ p > p1, \quad s_{in,j} \in S_{in,j}, \quad s_{out,j} \in S_{out,j}, \quad j \in J \qquad \text{(A.10)}$$

$$t_u\left(s_{in,j},p\right) \geq t_{out}\left(s_{out,j},p\right),$$
$$\forall p \in P, \quad s_{in,j} \in S_{in,j}, \quad s_{out,j} \in S_{out,j}, \quad j \in J \qquad \text{(A.11)}$$

Constraint (A.12) stipulates that a state can only be processed at a particular time point p in a particular unit j after it has been produced from another unit j'. In case of a recycle, j is the same as j'. It is worthy of note that constraints (A.11) and (A.12) are only applicable to intermediates, since they are the only states that are both produced and used.

$$t_u\left(s_{in,j},p\right) \geq t_{out}\left(s_{out,j'},p\right), \qquad \forall p \in P, \quad s_{out,j'} = s_{in,j}, \quad j, j' \in J \qquad \text{(A.12)}$$

Assignment constraint

Constraint (A.13) is the assignment constraint which is aimed at ensuring that only one task is conducted in a unit at any time point. It is therefore apparent that the assignment is only necessary if more than one task can be performed in a given unit. Otherwise, it is also redundant.

$$\sum_{s_{in,j} \in S_{in,j}} y\left(s_{in,j},p\right) \leq 1, \qquad \forall p \in P, \quad j \in J \qquad \text{(A.13)}$$

Time horizon constraints

Constraints (A.14) and (A.15), respectively, stipulate that the usage or production of a state should be within the time horizon of interest.

$$t_u\left(s_{in,j}, p\right) \leq H, \qquad \forall p \in P, \quad s_{in,j} \in S_{in,j}, \quad j \in J \qquad \text{(A.14)}$$

$$t_{out}\left(s_{out,j}, p\right) \leq H, \qquad \forall p \in P, \quad s_{out,j} \in S_{out,j}, \quad j \in J \qquad \text{(A.15)}$$

Storage constraint

Constraint (A.16) states that the amount of state s stored at each time point cannot exceed the maximum allowed.

$$q_s(s, p) \leq Q_s^U(s), \qquad \forall p \in P, \quad s \in S \qquad \text{(A.16)}$$

Appendix B: Scheduling model of Seid and Majozi (2012)

This scheduling framework also uses the state sequence network (SSN) recipe representation and an uneven discretisation of the time horizon with unit specific time points. The mixed integer linear programming (MILP) formulation can handle proper sequencing of tasks and accurately accounts for the fixed intermediate storage (FIS) operational policy. The model results in a reduction of event or time points required and as a result, gives better performance in terms of objective value and CPU time required when compared to previous literature models.

Allocation constraint

Constraint (B.1) ensures that only one task is performed in unit *j* at time point *p*.

$$\sum_{s_{in,j} \in S^*_{in,j}} y\left(s_{in,j}, p\right) \leq 1, \qquad \forall j \in J, \quad p \in P \tag{B.1}$$

Capacity constraint

Constraint (B.2) states that the total amount of all states consumed at time point *p* is limited by the capacity of the unit consuming the states. $V^L_{s_{in,j}}$ and $V^U_{s_{in,j}}$ represent the lower and upper capacity bounds for a unit which processes effective state $s_{in,j}$.

$$V^L_{s_{in,j}} y\left(s_{in,j}, p\right) \leq m_u\left(s_{in,j}, p\right) \leq V^U_{s_{in,j}} y\left(s_{in,j}, p\right),$$
$$\forall p \in P, \quad j \in J, \quad s_{in,j} \in S_{in,j} \tag{B.2}$$

Material balances for storage

Constraint (B.3) states that the amount of state *s* stored at time point *p* is equal to the amount stored at the previous time point adjusted by an amount which is the difference between the amount of state *s* produced at the previous time point (*p* - 1) and used by tasks at the current time point, *p*. This constraint is used for states other than products, as the latter are not consumed, but only produced.

$$q_s(s,p) = q_s(s,p-1) - \sum_{s_{in,j} \in S_{in,j}^{sc}} \rho_{s_{in,j}}^{sc} m_u(s_{in,j},p) + \sum_{s_{in,j} \in S_{in,j}^{sp}} \rho_{s_{in,j}}^{sp} m_u(s_{in,j},p-1),$$
$$\forall p \in P, \quad s \in S \tag{B.3}$$

Constraint (B.4) states that the amount of product stored at time point *p* is the amount stored at the previous time point added to the amount of product produced at time point *p*.

$$q_s(s^p,p) = q_s(s^p,p-1) + \sum_{s_{in,j} \in S_{in,j}^{s^p}} \rho_{s_{in,j}}^{sp} m_u(s_{in,j},p),$$
$$\forall p \in P, \quad s^p \in S^p \tag{B.4}$$

Duration constraint

Constraint (B.5) describes the duration of a task as a linear function of batch size. If the duration is not dependent on batch size, β is zero. For zero wait (ZW), only the equality sign is used.

$$t_p(s_{in,j},p) \geq t_u(s_{in,j},p) + \tau(s_{in,j})y(s_{in,j},p) + \beta(s_{in,j})m_u(s_{in,j},p),$$
$$\forall j \in J, \quad p \in P, \quad s_{in,j} \in S_{in,j} \tag{B.5}$$

Sequence constraints

Sequence constraints make sure that tasks are allocated correctly in a unit and ensure that the starting time of a new task is later than or equal to the finishing time of the previous task. Constraint (B.6) ensures the availability of units when the same task is performed in the same unit (the same state is used in the same unit). A state can only be used in a unit after all preceding tasks in the unit have been completed.

$$t_u\left(s_{in,j}, p\right) \geq t_p\left(s_{in,j}, p-1\right), \qquad \forall j \in J, \quad p \in P, \quad s_{in,j} \in S_{in,j}^{*} \tag{B.6}$$

Constraint (B.7) is similar to Constraint (B.6), but pertains to different tasks being performed in the same unit (different states used in the same unit). A task can only start in a unit after all previous tasks in the unit are complete.

$$t_u\left(s_{in,j}, p\right) \geq t_p\left(s_{in,j}^{'}, p-1\right),$$
$$\forall j \in J, \quad p \in P, \quad s_{in,j} \neq s_{in,j}^{'}, \quad s_{in,j}, s_{in,j}^{'} \in S_{in,j}^{*} \tag{B.7}$$

If a state is consumed and produced in the same unit and the produced state is unstable, Constraint (B.8) is used in addition to Constraint (B.7).

$$t_p\left(s_{in,j}^{usp}, p-1\right) \geq t_u\left(s_{in,j}^{usc}, p\right) - H\left(1 - y\left(s_{in,j}^{usp}, p-1\right)\right),$$
$$\forall j \in J, \quad p \in P, \quad s_{in,j}^{usc} \in S_{in,j}^{usc}, \quad s_{in,j}^{usp} \in S_{in,j}^{usp} \tag{B.8}$$

Constraints (B.9) to (B.12) are for different tasks that consume and produce the same state in different units. The starting time of the consuming task at time point p must be later than the finishing time of any task at the previous time point (p - 1), provided the state is used. Constraints (B.9) and (B.10) are used when an intermediate state s is produced from one unit.

$$\rho\left(s_{in,j}^{sp}\right)m_u\left(s_{in,j},p-1\right)\le q_s(s,p)+V_j^U tt(j,p),$$
$$\forall j\in J,\quad p\in P,\quad s_{in,j}\in S_{in,j}^{sp} \tag{B.9}$$

$$t_u\left(s_{in,j'},p\right)\ge t_p\left(s_{in,j},p-1\right)-H\left(2-y\left(s_{in,j},p-1\right)-tt(j,p)\right),$$
$$\forall j\in J,\quad p\in P,\quad s_{in,j}\in S_{in,j}^{sp},\quad s_{in,j'}\in S_{in,j}^{sc} \tag{B.10}$$

Constraint (B.9) states that if state *s* is produced from unit *j* at time point *p* - 1, but is not consumed at time point *p* by another unit *j'*, i.e. $tt(j,p)=0$, then the amount produced cannot exceed allowed storage, i.e. $q_s(s,p)$. However, if state *s* produced from unit *j* at time point *p* - 1 is used by another unit *j'*, then the amount of state *s* stored at time point *p*, i.e. $q_s(s,p)$ is less than the amount of state *s* produced at time point *p* - 1. The outcome is that the binary variable $tt(j,p)$ becomes 1 in order for Constraint (B.9) to hold. If the unit performs tasks like separation, distillation or other tasks that produce more than one intermediate at time point *p*, then the binary variable $tt(j,p)$ becomes $tt(j,s,p)$. This allows Constraint (B.10) to be relaxed for the unit that is not using the state produced by unit *j* at time point *p*. Simultaneously, for the other unit that uses the state produced by unit *j* at time point *p*, Constraint (B.10) holds.

Constraint (B.10) states that the starting time of a task consuming state *s* at time point *p* must be later than the finishing time of a task that produces state *s* at the previous time point *p* - 1, provided that state *s* is used. Otherwise this constraint is relaxed.

If an intermediate state is produced from more than one unit, Constraint (B.11) states that the amount of state *s* used at time point *p* can either come from storage or from other units that produce the same state, depending on the binary variable $tt(j,p)$.

$$\sum_{s_{in,j} \in S_{in,j}^{sc}} \rho_{s_{in,j}}^{sc} m_u(s_{in,j}, p) \leq q_s(s, p-1) + \sum_{s_{in,j} \in S_{in,j}^{sp}} \rho_{s_{in,j}}^{sp} m_u(s_{in,j}, p-1) tt(j, p),$$

$$\forall j \in J, \quad p \in P \qquad \text{(B.11)}$$

If the binary variable $tt(j, p)$ is 0, which means that state s produced from unit j at time point p - 1 is not used at time point p, then Constraint (B.10) is relaxed. If $tt(j, p)$ is 1, state s produced from unit j at time point p - 1 is used and Constraint (B.10) holds. Constraint (B.10) is therefore important both when a state is produced from one unit and when a state is produced from more than one unit. Although Constraint (B.11) is nonlinear, it can be linearised exactly using the Glover transformation (Glover, 1975).

Constraint (B.12) states that a consuming task can start after the completion of the previous tasks. Constraint (B.12) takes care of proper sequencing timing when a unit uses material which was previously stored. That is when the producing task is active at time point p - 2 and later produces and transfers the material to storage at time point p - 1. This available material in the storage at time point p - 1 is then used by the consuming task in the next time points. The starting time of the consuming task must therefore be later than the finishing time of the producing task at time point p - 2. Constraint (B.10) is used for proper sequencing if the amount of material used by the consuming task at time point p is currently produced by the producing units. Consequently, Constraint (B.12) together with Constraint (B.10) results in feasible sequencing time when the consuming task uses material which was previously stored and/or material which is currently produced by the producing units.

$$t_u(s_{in,j'}, p) \geq t_p(s_{in,j}, p-2) - H(1 - y(s_{in,j}, p-2)),$$

$$\forall j \in J, \quad p \in P, \quad s_{in,j} \in S_{in,j}^{sp}, \quad s_{in,j'} \in S_{in,j'}^{sc} \qquad \text{(B.12)}$$

Sequence constraints for FIS policy

In most previous scheduling formulations, proper modelling for finite intermediate storage has been overlooked, which results in unlimited intermediate storage (UIS) behaviour. Constraints (B.13) and (B.14) address this. A new binary variable $xx(s,p)$ is introduced which indicates the availability, $xx(s,p)=1$ and absence, $xx(s,p)=0$, of storage. Constraint (B.13) states that any state *s* can only be stored if the capacity of available storage will not be exceeded. Otherwise, state *s* will either be produced and consumed immediately or not produced at all. Constraint (B.14) enforces this condition.

$$\sum_{s_{in,j}\in S_{in,j}^{sp}} \rho_{s_{in,j}}^{sp} m_u(s_{in,j}, p-1) + q_s(s, p-1) \le Q_s^U + \sum_{j\in J_s} V_j^U (1 - xx(s,p)),$$
$$\forall j \in J, \quad p \in P, \quad s \in S \qquad \text{(B.13)}$$

$$t_u(s_{in,j'}, p) \le t_p(s_{in,j}, p-1) + H(2 - y(s_{in,j'}, p) - y(s_{in,j}, p-1)) + H(xx(s,p)),$$
$$\forall j \in J, \quad p \in P, \quad s_{in,j} \in S_{in,j}^{sp}, \quad s_{in,j'} \in S_{in,j}^{sc} \qquad \text{(B.14)}$$

According to Constraint (B.14), the starting time of a task that consumes state *s* at time point *p* must be equal to the finishing time of a task that produces state *s* at time point *p* - 1, if both consuming and producing tasks are active at time point *p* and time point *p* - 1, respectively and if there is no storage to store the amount of state *s* produced at time point *p*. In a case when storage is available to store a state *s* at time point *p*, then the starting time of the consuming task at time point *p* is not necessarily equal to the finishing time of a task producing state *s* at time point *p* - 1. Constraints (B.13) and (B.14) reduce the number of time points and give a better objective value.

Storage constraints

Constraint (B.15) indicates that the amount of state s stored at any time point must not exceed the maximum capacity of available storage. State s that is produced at time point p - 1 can be stored for a while in a unit that is producing it in the next time points until it is used, if the unit is not performing tasks.

$$q_s(s,p) \leq Q_s^U + \sum_{s_{in,j} \in s_{in,j}^{sp}} uu(s_{in,j}, p), \qquad \forall s \in S, \quad p \in P, \quad j \in J \qquad \text{(B.15)}$$

Constraint (B.16) states that a portion of the state that is produced at time point p can be stored in the unit for consecutive time points, if the unit is not active in those consecutive time points. This is a similar concept to that of slot based formulations that allow tasks to continue in the next consecutive slots, indicating that the unit stores the states in those consecutive time points.

$$uu(s_{in,j}, p) \leq \rho_{s_{in,j}}^{sp} m_u(s_{in,j}, p-1) + uu(s_{in,j}, p-1), \qquad \forall p \in P, \quad j \in J \qquad \text{(B.16)}$$

Constraint (B.17) ensures that if a state is stored at time point p in the unit then the unit should not be active to start any other task.

$$uu(s_{in,j}, p) \leq V_j^U \left(1 - \sum_{s_{in,j} \in S_{in,j}^*} y(s_{in,j}, p) \right), \qquad \forall p \in P, \quad j \in J \qquad \text{(B.17)}$$

Time horizon constraints

The usage and production of states should be within the time horizon of interest. These conditions are expressed in Constraints (B.18) and (B.19).

$$t_u\left(s_{in,j},p\right)\le H, \qquad \forall s_{in,j}\in S_{in,j}, \quad p\in P, \quad j\in J \tag{B.18}$$

$$t_p\left(s_{in,j},p\right)\le H, \qquad \forall s_{in,j}\in S_{in,j}, \quad p\in P, \quad j\in J \tag{B.19}$$

Tightening constraints

Constraint (B.20) is used to tighten the model. The sum of the durations of all tasks in a unit must be within the time horizon.

$$\sum_{s_{in,j}\in S^{*}_{in,j}}\sum_{p}\left(\tau\left(s_{in,j}\right)y\left(s_{in,j},p\right)+\beta\left(s_{in,j}\right)m_u\left(s_{in,j},p\right)\right)\le H, \quad \forall p\in P, \quad j\in J \tag{B.20}$$

Objective function

The objective of a scheduling problem is to maximise the product throughput if the target is not known *a priori* or to minimise the makespan if the target is known beforehand, as given in Constraint (B.21).

$$\text{maximise}\sum_{s}CP\left(s^{p}\right)q_s\left(s^{p},p\right), \qquad \forall p=P, \quad s^{p}\in S^{p}$$

or

$$\text{minimise}\, H \tag{B.21}$$

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