UNIVERSITY OF THE
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JOHANNESBURG

HEAT INTEGRATION OF MULTIPURPOSE BATCH PLANTS THROUGH MULTIPLE HEAT STORAGE VESSELS

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Master of Science in Engineering by research:

“A dissertation submitted to the Faculty of Engineering and Built Environment,
University of the Witwatersrand, Johannesburg, in fulfilment of the
requirements for the degree of Master of Science in Engineering.”

Johannesburg, 05 February 2018

DECLARATION:

I declare that this dissertation is my own unaided work. It is being submitted for the Degree of Master of Science in Chemical Engineering to the University of the Witwatersrand, Johannesburg. It has not been submitted before for any degree or examination to any other University.

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(Signature of Candidate)

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ACKNOWLEDGEMENTS

First and foremost I would like to thank my Lord Jesus. I would not be where I am today without my Lord.

Thank you to my professor and mentor in many ways, Professor Thokozani Majozi for his guidance, support and for always challenging me to be and do better.

Thank you to the Sustainable Process Engineering team for the support and the encouragement always. A special appreciation goes to Christie Bazolona and Thabang Kgongwana for their immense help during my time doing my Master’s degree. I would also like to thank my family for their endless love and support at all times, and my colleagues at AEL Mining Services for their support during the last days of writing my dissertation.

Thank you to the National Research Foundation (NRF) and AECI for funding my Masters research.

SYNOPSIS

In most industrial processes, energy is an integral part of the production process; therefore, energy consumption has become an intensified area in chemical engineering research. Extensive work has been done on energy optimisation in continuous operations; unlike in batch operations because it was believed that due to the small scale nature of batch plants, small amounts of energy is consumed. Certain industries such as the brewing and dairy industries have shown to be as energy intensive as continuous processes. It is, therefore, necessary for energy minimisation techniques to be developed specifically for batch processes in which the inherent features of batch operations such as time and scheduling are taken into account accordingly. This can be achieved through process integration techniques where energy consumption can be reduced while economic feasibility is still maintained. Most of the work done on energy minimisation either focuses on direct heat integration, where cold and hot units operating simultaneously are integrated, or indirect heat integration, where units are integrated with heat storage. The schedules used in these models are, in most cases, predetermined which leads to suboptimal results.

This work is aimed at minimising energy consumption in multipurpose batch plants by using direct heat integration together with multiple heat storage vessels through mathematical programming. The proposed approach does not use a predetermined scheduling framework. The focus lies on the heat storage vessels and the optimal number of heat storage vessels together with their design parameters, namely size and the temperature at which the vessels are initially maintained, are determined.

The formulation developed is in the form of a mixed integer non-linear program (MINLP) due to the presence of both continuous and integer variables, as well as non-linear constraints governing the problem. Two illustrative examples are applied to the formulation in which the optimal number of multiple heat storage vessels is not known beforehand. The results rendered from the model show a decrease in the external utilities, in the form of cooling water and steam, compared to the base case where no integration is considered and the case where only one heat storage vessel is used.

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CHAPTER 1

INTRODUCTION

1.1.Background

The use of batch chemical processes has gained popularity in South Africa, due to their use in the production of low volume and high value products in the pharmaceutical, food, explosives, and specialty chemicals industries (Seid & Majozi, 2012).. Due to the rising growth in the use of batch chemical processes, research and developments in the area have been intensified in order to develop optimisation methods that can be used to operate the processes at optimal conditions. In the past the focus has been on design methods that are aimed at minimising the capital investment based on the selection of capital equipment. The focus has since shifted to optimisation methods that include those that can reduce operating costs, such as utility costs by reducing the energy requirement in the process (Bieler, 2004).

In most industrial processes, energy is an integral part of the production processes, therefore, energy consumption has become an intensified area in chemical engineering research. Extensive work has been done on energy optimisation in continuous operation, unlike in batch operations. It is important to emphasise that it was believed that due to the small scale nature of batch plants, small amounts of energy is consumed. Certain industries such as the brewing and dairy industries have shown to be as energy intensive as continuous processes (Seid & Majozi, 2014). It is, therefore, necessary for energy minimisation techniques to be developed specifically for batch processes in which the inherent features of batch operations such as time and scheduling are taken into account accordingly.

Optimisation has been used as a way of minimizing energy in both batch and continuous operations. There are two main ways in which energy minimisation in batch plants has been studied and conducted, namely; pinch analysis or graphical techniques and mathematical optimisation. Some heuristics methods have also been developed in minimising energy, but do not constitute as the majority of the methods developed. Graphical techniques have been applied by modifying pinch analysis to suit batch process. The first work reported was by Clayton (1986) where the time average model was introduced to minimise energy consumption while considering the time characteristic of batch processes. Recently the work of Chaturvedi & Bandyopadhyay (2014) presented a methodology where pinch analysis was used. The aim of the study was to find the minimum utility requirements of a batch process with a fixed schedule.

Mathematical optimisation presents a way in which the schedule of the batch process together with several utilities such as energy can be optimised simultaneously or individually. The optimisation of energy in batch processes can be categorized into two groups, i.e. direct heat integration and indirect heat integration. Direct heat integration is minimising energy consumption by using heat given off from one unit in the process to heat up another unit. This was demonstrated by the work done by Majozi (2006) where only direct heat integration was considered. Indirect heat integration is the use of heat storage vessels to heat or cool units in the process, depending on the temperature requirements of the units and was illustrated by De Boer et al. (2006). An illustration of direct and indirect heat integration is shown in Figure 1.1 where H is the time horizon. Most of the work done on heat integration either focuses on direct heat integration or indirect heat integration. A combination of direct and indirect heat integration has also been explored in literature such as the work by (Ivanov, et al., 1992; Majozi, 2009; Seid & Majozi, 2014)

Energy optimisation of batch processes through heat integration requires scheduling considerations. Scheduling describes the order in which tasks are performed in the plant together with the time requirement of the task i.e. starting and finishing times as well as the quantity of the tasks (Seid & Majozi, 2012). There are two types of schedules that can be used in batch processes, predetermined and variable schedules. Predetermined schedules describe an order of processing tasks with known starting and finishing times before any optimisation technique is applied to the process. Variable schedules are those that are embedded in the heat integration mathematical model and are simultaneously optimised with the integration model in order to obtain the optimal schedule of the process. In most cases, predetermined schedules, when used as the platform to optimise the energy consumption in a plant, lead to suboptimal results.

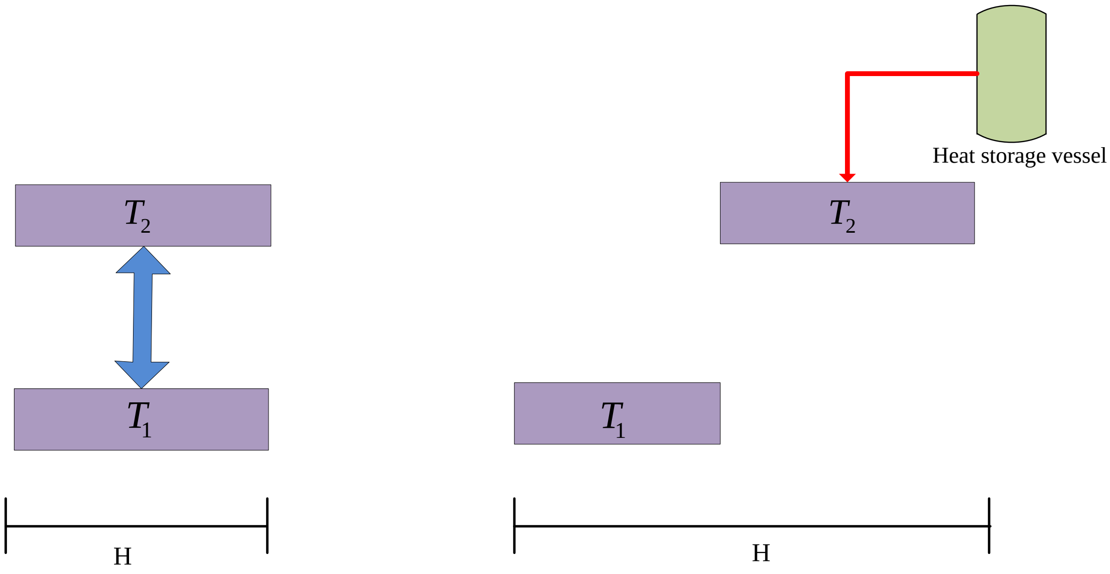

Figure 1.1: Types of heat integration in batch processes

In this body of work, mathematical optimisation is used to optimise the schedule of batch processes together with energy requirement of the plant. Most of the work done on heat integration either focuses on direct heat integration or indirect heat integration. The schedules used in these models are, in most cases, predetermined which can lead to suboptimal results. In the proposed formulation, simultaneous optimisation of the schedule and heat integration is carried out by using the schedule as a foundation of the model and adding the heat integration techniques. The objective function of the schedule is then combined with the heat integration objective function and the two models are solved as one, as shown in Figure 1.2. The paper proposes a novel mathematical formulation based on the design of multiple heat storage vessels, where the operation of heat transfer between units and the heat storage vessels are adequately taken into account by allowing the time of heat transfer to coincide with the task duration.

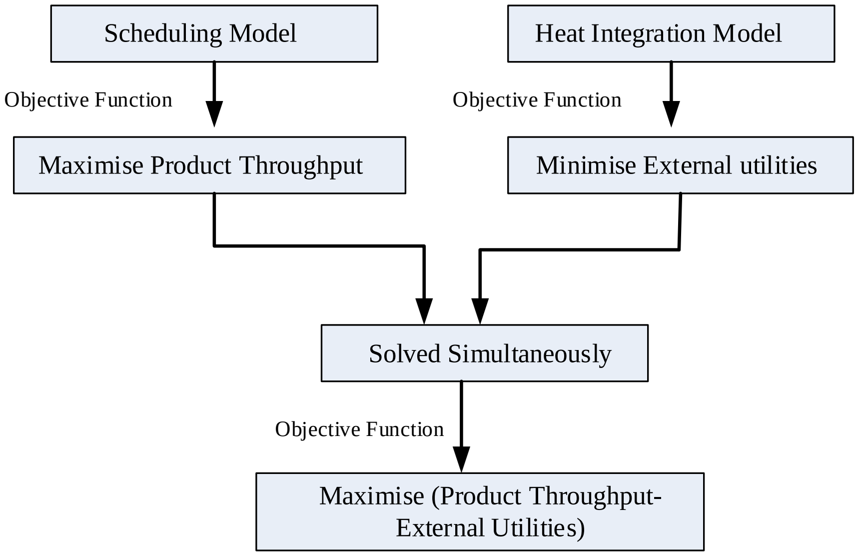

Figure 1.2: Flowchart for proposed formulation

1.2. Motivation

The objective of most mathematical models used in energy optimization of batch plants is to maximise profits by maximising throughput while minimising utility costs. The nature of batch processes makes it possible that there could simultaneously be a task in the process that needs heating, s_{jc}^{in} and another task that needs cooling s_{jh}^{in}, as shown in Figure 1.3(a). Traditionally, this occurrence would provide an opportunity for process-process heat integration, if the thermal driving forces allow. However, if the thermal driving forces do not allow, heat storage provides another viable option towards energy minimisation. There are two scenarios that could occur, should there only be one heat storage vessel available in the plant. One of the tasks could be integrated with the heat storage vessel while the other is supplied by external utilities in order for its temperature requirement to be satisfied. This describes the first scenario depicted in Figure 1.3(b). The second scenario is when one task is integrated with the storage vessel and the other task is delayed for later into the time horizon so that it could be integrated with the same heat storage vessel once the latter is available for integration, as illustrated in Figure 1.3(c). Clearly, this would ultimately reduce the number of batches which could be processed within the given time horizon. This drawback could be avoided by using multiple heat storage vessels that could allow for multiple heat integration between processing tasks and heat storage units in a situation where heating and cooling are required simultaneously as aforementioned. This is shown in Figure 1.3(d). Almost invariably, this option would allow more batches to be produced within the time horizon of interest, whilst taking advantage of available heat in the process. Consequently, this contribution is aimed at determining the optimum number, size and thermal profiles of heat storage vessels to achieve minimum energy use in multipurpose batch plants.

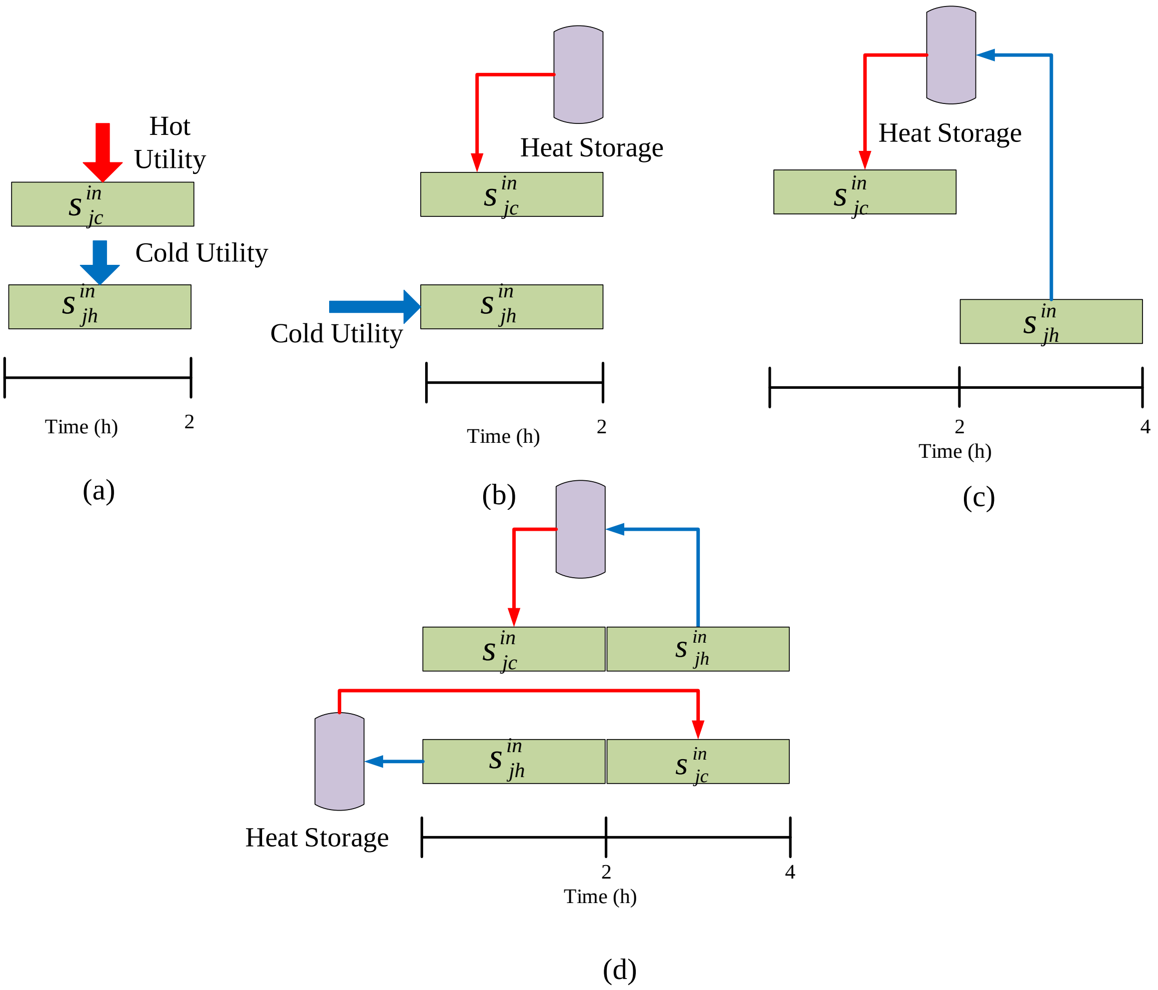

Figure 1.3: (a) Tasks requiring heating/cooling, (b) scenario using one heat storage vessel, (c) scenario using one heat storage vessel and (d) scenario using multiple heat storage vessels

1.3. Objectives

The objectives of the study can be summed up as follows:

i. To develop a heat integration framework for batch plants which takes into account direct and indirect heat integration and includes multiple heat storage vessels
ii. To embed a scheduling framework within the heat integration framework
iii. To simultaneously optimise the schedule and the heat integration model
iv. To determine the heat network of the plant

v. To design the storage vessels

1.4. Problem Statement

The problem addressed in this work can be stated as follows:

Given:

i. Production scheduling data including duration of tasks, capacities of processing units, storage capacities, product recipe and time horizon,
ii. Supply and target temperatures of hot and cold tasks,
iii. Specific heat capacities of hot and cold states,
iv. Cost of hot and cold utilities,
v. Minimum allowable temperature difference,
vi. Size limits for the heat storage vessels and temperature limits for the initial temperature of the heat storage vessels, and
vii. Cost parameters of the heat storage vessels.

Determine:

i. An optimal production schedule where the objective is to maximise profit,
ii. The optimal number of heat storage vessels with their respective optimal sizes and initial temperatures.
iii. The temperature profiles of the heat storage vessels

1.5. Structure

Chapter 2 gives a detailed literature of heat integration in multipurpose batch processes where basic concepts of process integration and batch processes are introduced, and scheduling and heat integration techniques are outlined. The mathematical model is given in chapter 3 with a full description of the constraints and objective function used. Two illustrative examples were studied and analysed and the results and discussion are given in chapter 4. Chapter 5 gives a description of the recommendations and considerations for future work and chapter 6 outlines the conclusions of the study. All chapters include references at the end of the chapter.

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CHAPTER 2

LITERATURE REVIEW

2.1. Introduction

In order to obtain a full appreciation of batch process, their intricate nature and the way in which energy minimisation can be applied, a comprehensive literature review is presented. The basic concept of process integration is outlined where the different techniques of process integration are discussed. An overview of batch processes, detailing the unique characteristics, are discussed where the types of batch processes, time, operational philosophies, recipe representation and the scheduling techniques are outlined.

The last section looks at heat integration. The different methods of optimising energy usage in batch processes are explored by detailing the pinch analysis methodology, mathematical optimisation as well as heuristics and hybrid methods which are a combination of the different types of energy optimisation methods.

2.2. Process integration

Energy minimisation can be achieved through the use of process integration. El-Halwagi (1997) describes process integration as “a holistic approach to process design, retrofitting and operation of existing plants which emphasises the unity of the process and considers the interactions between different unit operations from the outset rather than optimising them separately”. Optimisation is essential in chemical engineering processes because it is used for the improvement of initial design of equipment. Optimisation also facilitates enhancements in the operation of the equipment once the equipment is installed, in order to realise the largest production, the greatest profit, the minimum cost, the least energy usage and so on (Edgar & Himmelblau, 1988).There are three steps that should be followed for process integration according Mann (1999).

i. The overall process must first be considered as one integrated system of process units that also includes waste and utility streams.
ii. Process-engineering techniques are then applied to the system. These techniques can include thermodynamics, mass and energy balances.

iii. The resultant design or synthesis of the plant can then be finalized, depending on the process-engineering techniques which were applied to the plant.

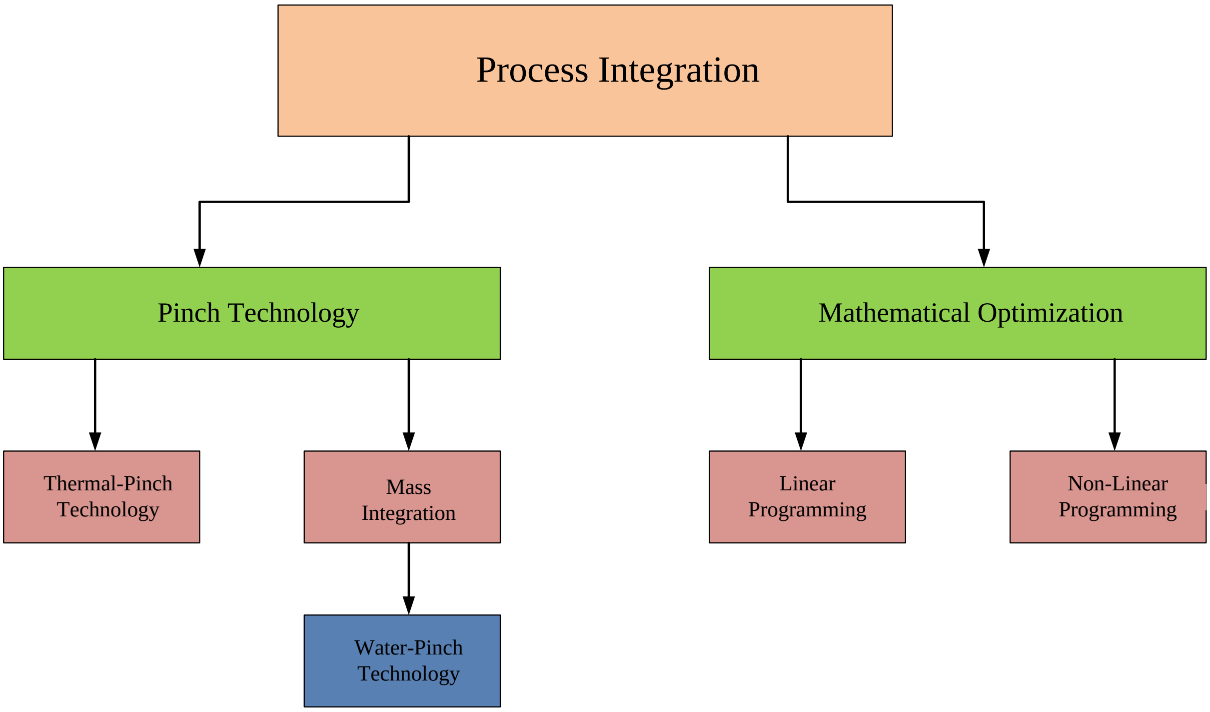


Figure 2.1: Flow diagram for process integration

Process integration can be achieved through two techniques i.e. pinch technology (graphical-based optimisation) and mathematical optimisation. Pinch technology includes the consideration of thermal-pinch technology and mass integration which primarily considered water-pinch technology. Mathematical optimisation can be separated into linear and non-linear programming (Mann, 1999). The flow diagram of process integration is shown in Figure 2.1. Optimisation in process plants can also be based on heuristics by using experience to improve plant performance.

2.2.1. Pinch analysis (Graphical optimisation)

Graphical optimisation techniques can be employed through pinch analysis, which was initially applied in energy minimisation methods in continuous processes. Linhoff (1998) defines pinch technology as a form of process integration technique that uses thermodynamics principles to systematically obtain the minimum energy usage of a process. Pinch analysis has since been adapted and used for energy minimisation in batch processes. It has also been used in mass integration such as materials recycling, waste minimisation and reducing external separating agents Gadalla (2015). Pinch analysis is characterised by the use of hot and cold composite curves. Composite curves are used to show heat availability, streams that need cooling and heat demands, streams that need heating, for energy minimisation or fresh water requirement and wastewater reuse for wastewater minimisation (Wang & Smith, 1995). After the construction of the hot and cold composite curves, the energy or mass recovery for the process can be determined by overlapping the composite curves as shown in Figure 2.2. The resultant diagram shown in Figure 2.3 indicates that the remaining heating and cooling needs are the minimum hot utility requirement $(Q_{H\min})$ and the minimum cold utility requirement $\left(Q_{C\min}\right)$ (Linhoff, 1998). The pinch is also shown in Figure 2.2. The system above the pinch is a heat sink, where heat is required and the system below is the heat source, where heat is given off. The same concept of using composite curves is used for mass integration, although other considerations are taken into account depending on the type of mass integration taking place. In the instance where wastewater minimisation is being conducted, the flowrate and concentration of the wastewater is considered.

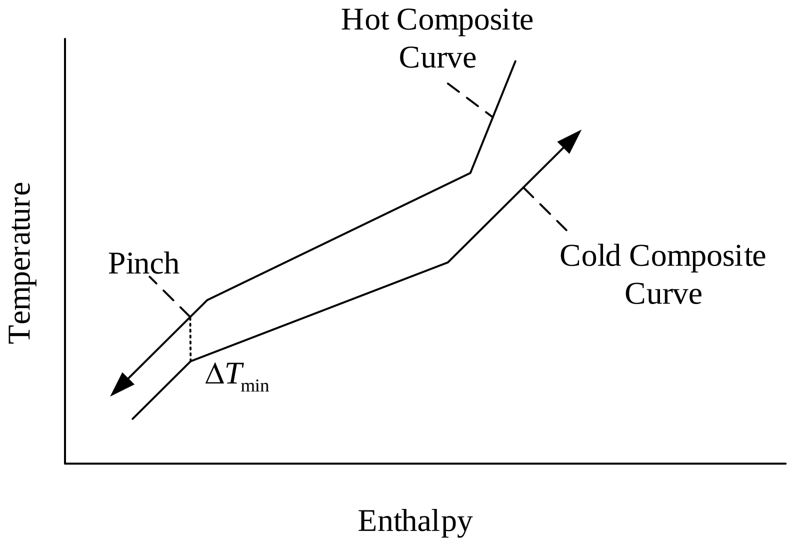


Figure 2.2: Composite curves for pinch analysis

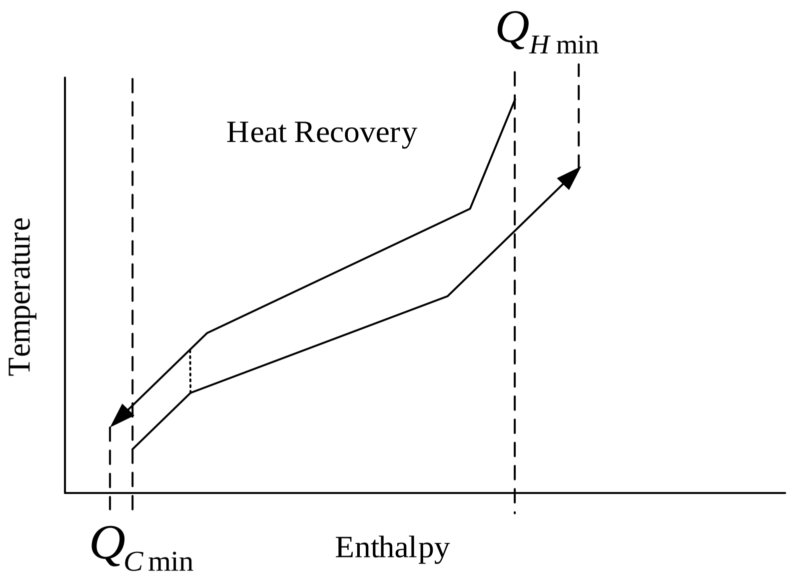


Figure 2.3: Composite curve for pinch analysis

2.2.2. Mathematical optimisation

Mathematical optimisation can be defined as “the science of determining the best solutions to mathematically defined problems, which may be models of physical reality or of manufacturing and management systems” according to Synman (2005) A process can be defined by a set of equations or experimental data. A performance criterion such as maximisation of profit or minimisation of operating costs can then be used to determine how the process is performing. Mathematical optimisation techniques can be used to determine the values of operating variables that give the best value for the performance criterion (Edgar & Himmelblau, 1988) .

For every optimisation problem, there are three essential features which must exist. These features are outlined as follows:

i. Minimum of one objective function
ii. Equality constrains
iii. Inequality constraints

The optimisation problem is then described in the following format:

Minimize: $f(x)$ (objective function)

Subject to: $h(x) = 0$ (equality constraint)

$g(x) \geq 0$ (inequality constraint)

Where x is a vector of variables, and $h(x)$ and $g(x)$ are vectors of equations. Figure 2.4 shows the linear equality constraints as well as the non-linear inequality constrains as a general example of an optimisation problem. The graph in Figure 2.4 also shows the feasible region which is the region of all the feasible solutions defined by the constraints. A feasible solution can then be found in the feasible region which is a set of variables that satisfies the constraints of the problem (Edgar & Himmelblau, 1988). The feasible solution can be an optimal solution which means not only does the set of variables found that satisfy the constraints, but the set of variables found give the best solution for the objective function.

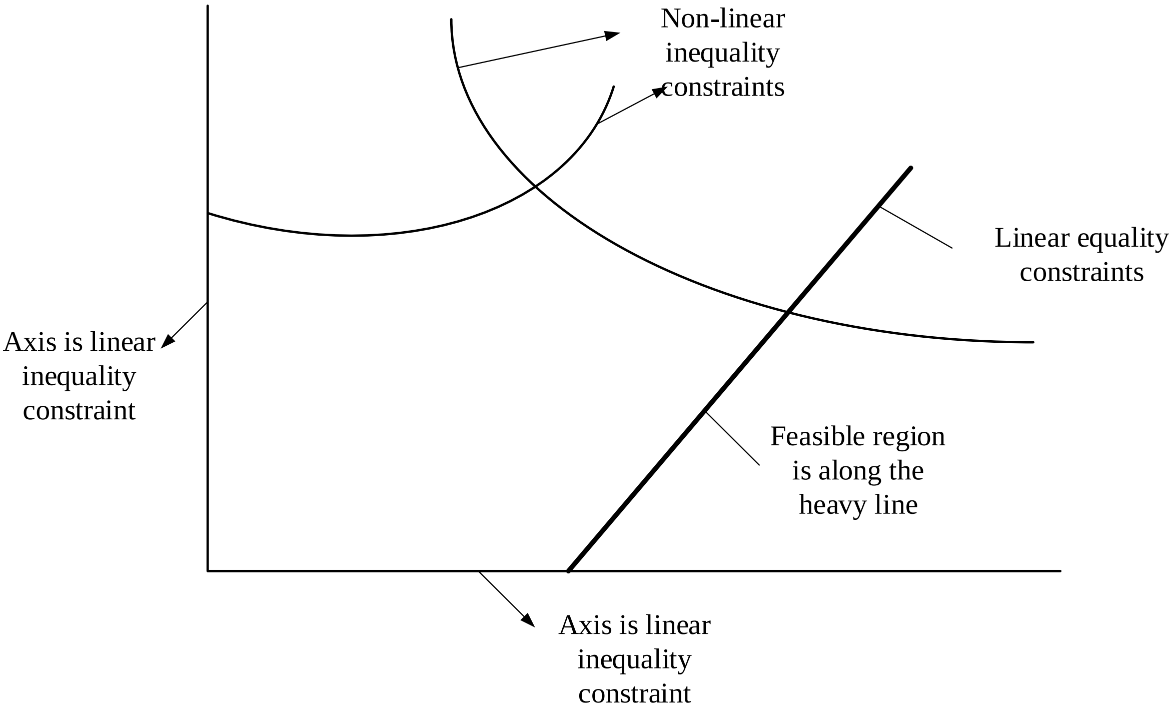


Figure 2.4: Mathematical optimisation illustration (Edgar & Himmelblau, 1988)

2.2.3. Heuristics

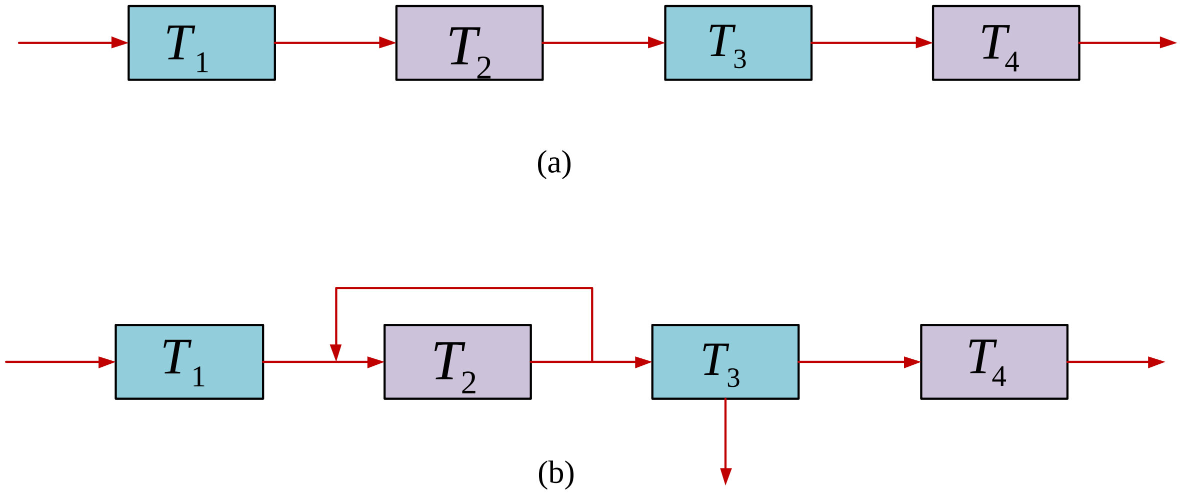
Process integration has also been conducted by employing heuristics as a technique (Vaselenak et al., 1986). Heuristics can be defined as the use of experience to learn and improve. This form of technique is used readily in industry as most optimisation methods done on processes are based on what is already known. This means that what has been done before is used as information to optimise processes and units. This form of optimisation technique can mainly be done on a certain number of equipment and not necessarily the whole plant or process.

The different types of process integration techniques are applied differently depending on the type of process that is being optimised. It is thus necessary to understand the fundamentals of batch processes and the way that the process integration techniques are adapted in order to achieve optimal operating conditions.

2.3. Batch processes

Processes that comprise of temporary discrete tasks that must be undertaken in order to produce final products from raw materials are called batch processes. The quantity of materials to be processed and the duration of the tasks must be clearly stipulated. The sequence of tasks to be followed in order for the final products to be produced must also be known. Batch processes are, in most instances, used in specialty chemicals production, pharmaceuticals and brewing. This is mainly due to the types of products that are produced from these industries, which are of high quality products at lower volumes compared to continuous processes (Rippin, 1983). Due to the increasing use of batch processes, it is vital to know and understand the core functionalities of batch processes in order to increase their operational efficiencies.

There are two types of batch processes, namely, multiproduct batch processes and multipurpose batch processes. Rippin (1983) defines a multiproduct process as one in which a number of products are produced successively in a sequence of single product campaigns where each product follows only one route as shown in Figure 2.5a. Multipurpose batch processes are defined as processes which produce multiple different products at the same time as depicted in Figure 2.5b. The same product can be produced in one plant through different routes in the process.



(a)

(b)

Figure 2.5: Types of batch processes

The main characteristic of batch plants is in their dependence on time, unlike continuous operations, which can operate at steady state. In batch processes, there are starting times and finishing times for all tasks. Tasks can produce intermediate material that must be used as a raw material for a subsequent task. Therefore, time must be addressed adequately in the batch processes in order for the correct operational sequence to be obtained. This is depicted in the Figures 2.6 and 2.7 below as adapted from Majozi (2010).

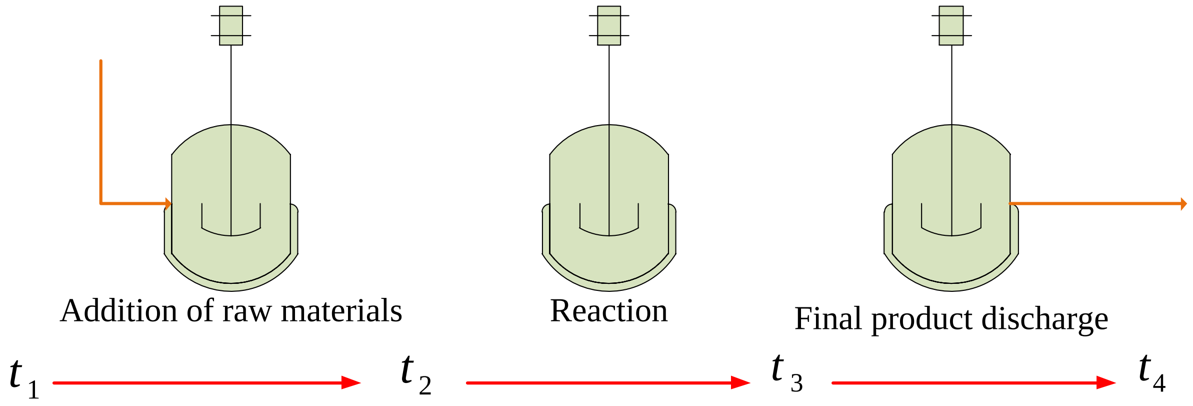


Figure 2.6: Batch reaction. Adapted from Majozi (2010)

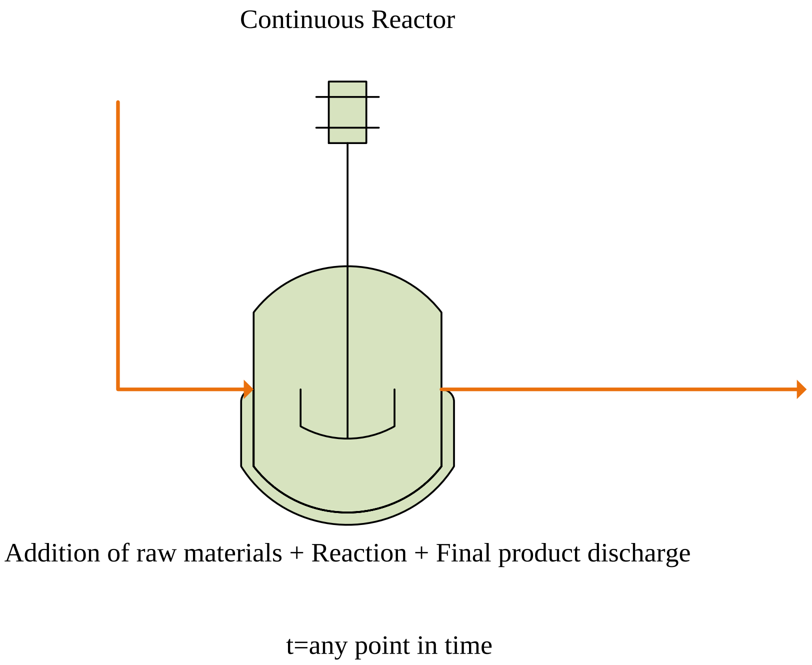


Figure 2.7: Continuous reactor. Adapted from Majozi (2010)

2.4. Capturing time

In batch processes, it is important to capture the essence of time in its exact nature unlike in continuous processes, where time is overridden. In literature, there exist three types of methods in which time is defined according to Majozi (2010). These include time average models (TAMs) which treat batch processes as pseudo-continuous operations. The second type of method tends to treat time as a fixed parameter that is known a priori with no opportunity for variance of the time horizon. Lastly, time can be treated in its exact manner by allowing time to vary in search of the true optimum. The variable time models can be categorised in precedence based models and time grid models. The flow diagram of time models is given in Figure 2.8.

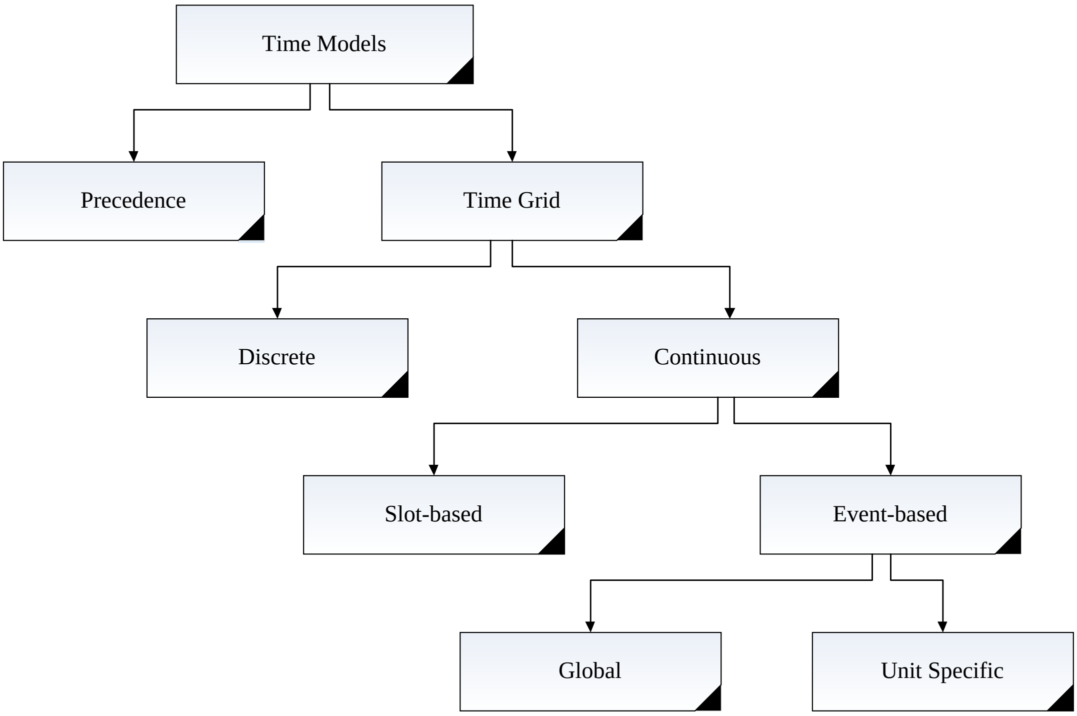
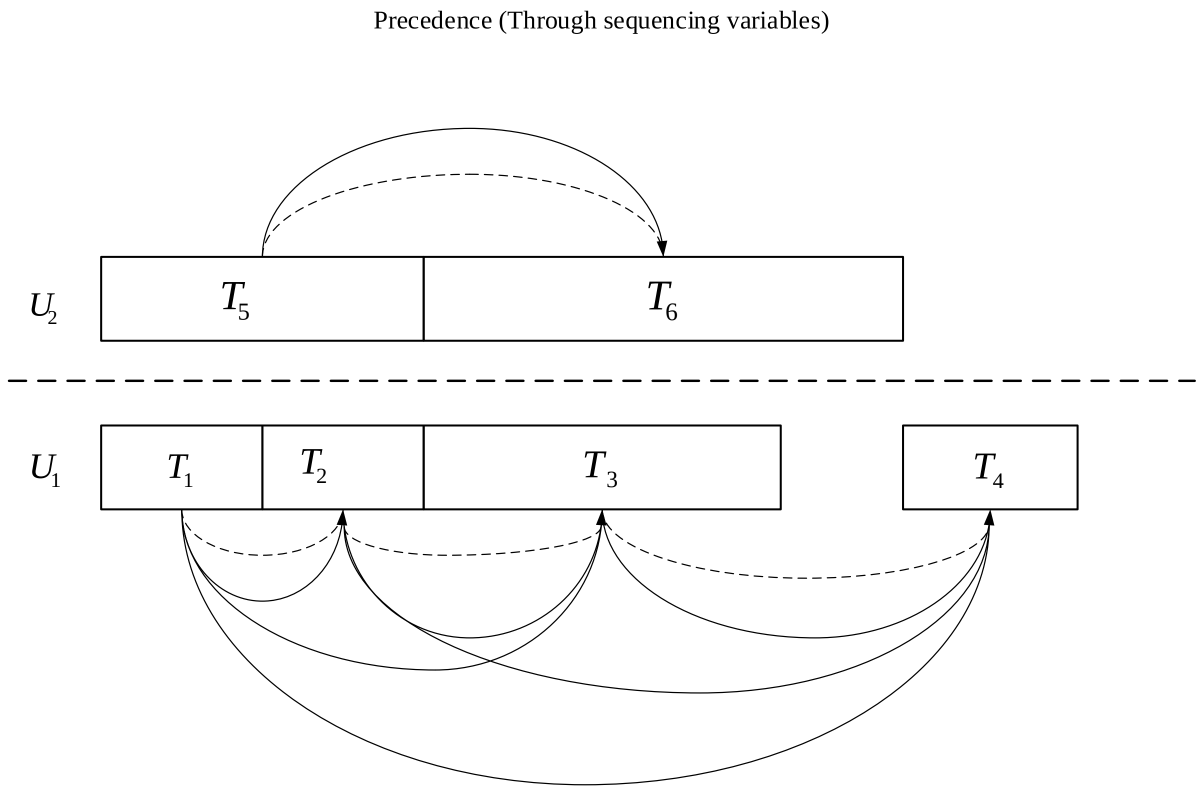


Figure 2.8: Flow diagram for time models

2.4.1. Precedence models

Time models that include unit-batch allocation and batch-batch sequencing are defined by Pinto and Grossmann (1998) as precedence based models. Harjunkoski et al. (2014) state that these models are mainly used for the scheduling of sequential environments such as multiproduct batch processes. Unit-batch allocation is modelled by taking into account binary variables which assigns a specific batch to a specific unit and constraints that ensure that for any one unit at a particular stage, only batch can be assigned to the unit. In order for one batch to be processed in one unit at a stage, sequencing constraints are used. Sequencing constraints are modelled using two types of precedence variables namely; intermediate and global precedence variables. The intermediate precedence variable is used when a certain batch immediately follows another batch and the global precedence variable is used for when a specific batch follows another batch but not necessarily immediately after. The precedence model is shown in Figure 2.9.



Precedence (Through sequencing variables)

Figure 2.9: Illustration of precedence models (Hajunkoski, et al., 2014)

2.4.2. Time-grid-based models

Time grid models are all the models that describe time using slots, periods, points or events. According to Harjunkoski et al. (2014), time-grid-based models rely on mapping of tasks onto one or more time reference grids. The models can further be categorised into two main groups; discrete-time models and continuous-time models depicted in Figures 2.10 and 2.11.

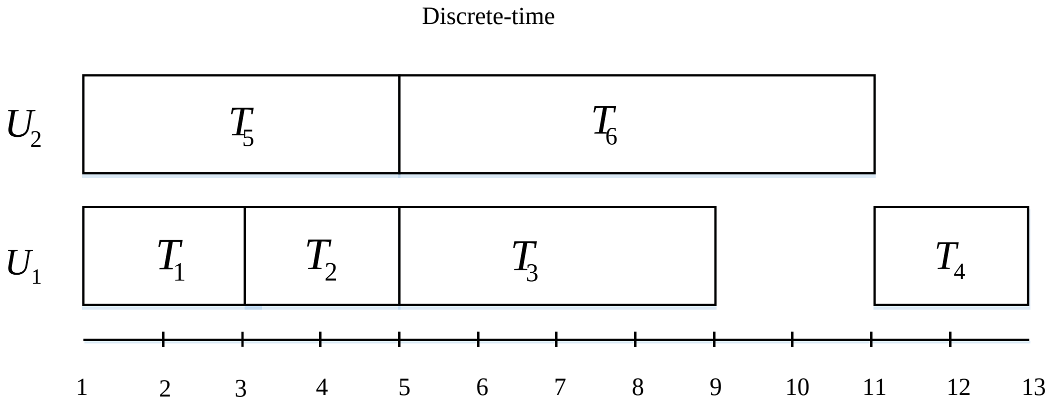


Figure 2.10: Discrete time model. Adapted from Harjunkoski et al. (2014)

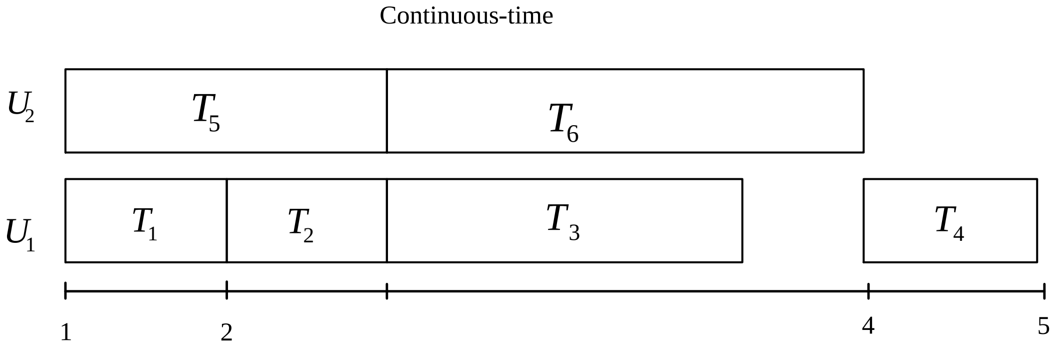


Figure 2.11: Discretization of time. Adapted from Harjunkoski et al. (2014)

a) Discrete time

The definition of discrete time representation is when the time horizon is divided into intervals of the same length. The event of the tasks such as starting and finishing times will coincide with the boundaries of the intervals. Discrete time representation is a simpler way of representing time due to its ability to provide a reference grid for all operations competing for shared resources such as equipment (Floudas & Xiaoxia, 2004). The duration of a time interval is taken as the highest common factor of the processing times given in the problem (Kondili, et al., 1993). In order for the model to be accurate, intervals of smaller sizes will be required which results in large models due to the large number of intervals. The duration of the tasks should also be in multiples of the length of the time intervals. (Hajunkoski, et al., 2014).

b) Continuous time representation

Due to the limitations of discrete time representations, continuous-time models were introduced. Continuous-time models, also known as uneven time discretization, are partitioned into a fixed number of time periods, whose length is determined by the optimization model (Hajunkoski, et al., 2014). This discretization of time is applied by only using the necessary number of time points corresponding to beginning and ending of tasks (Ierapetritou & Floudas, 1998). There are three types of continuous time representation, namely, slot-based models, global event-based models and unit specific event-based models.

Slot-based models

Slot-based models are those that have the time horizon represented in ordered blocks of unknown length which are also called variable length slot according to Shaik & Floudas (2008). The starting and finishing times of a task are then denoted by the boundaries of the variable length slot. The boundary of a finishing time can also be the boundary of starting time of a subsequent task. This helps in the reduction of the total number of slots for the problem.

Global event-based models

The global event-based models are those that use time points also known as event points to denote specific points in time that are used for all units and for all tasks. Floudas & Xiaoxia (2004) described global event based models as models which introduce continuous variables to determine the timings of events or variable time slots and use binary variables to assign important state changes, for example, the start or end of task, to these events or time slots. The seminal work reported on continuous time scheduling models using global event-based time representations was reported by Zhang & Sargent (1996; 1998). The formulation indicated that the most important variables for this specific type of time representation include:

- Timing event which is a continuous variable
- Binary variable indicating the existence or non-existence of a task i.e. starting time

- Binary variable indicating a specific starting time of a task in a unit that completes at a specific time

Unit specific event-based models

Unit specific event-based time representation differ from global event-based time representation in that the location of the event point differ for each unit. This allows different tasks to start at different moments in different units for the same event points as stated by Floudas & Xiaoxia (2004). Due to this definition of unit specific event-based models, adequate sequence constraints need to be added to the formulation in order for the timings of the tasks to be accurately captured. Another definitive characteristic of unit specific event-based time models is that unlike global event-based models, the event is defined as the starting of a task only instead of both the starting and finishing of the task. This results in the reduction of binary variables. The important variables taken into account in this formulation as described by Floudas & Xiaoxia (2004) include:

- Binary variable which determines whether or not a specific task starts at a specific event point
- Binary variable to determine whether or not a specific unit starts being utilized at a specific event point

Due to the time restriction in batch processes, storage becomes an important aspect. Intermediates must be stored in most instances, therefore the time of storage, capacities storage and the type of intermediate must be taken into account. These storage considerations are called operational philosophies.

2.5. Operational philosophies

Different kinds of operational philosophies that can be applied to different batch processes, depending on the kind of storage the process requires. Majozi (2010) gave a brief discussion on these operational philosophies. In processes where the product is retained in the processing unit before further processing; the no intermediate storage (NIS) operational philosophy is applied, shown in Figure 2.12. NIS is normally applied in processes where the space for storage tanks is not available. In instances where the product cannot be stored in its processing unit, intermediate storage is required. Intermediate storage is used in order to introduce flexibility to the process, in the sense that once a unit has completed a task, the material can be stored in a storage tank, making the unit available to perform the next task. The type of intermediate storage that is used depends on the nature of the process. The different types of intermediate storage philosophies that can be applied are finite intermediate storage (FIS), unlimited intermediate storage (UIS), common intermediate storage (CIS), mixed intermediate storage (MIS), process intermediate storage (PIS), zero wait (ZW), unlimited wait (UW) and finite wait (FW). Majozi (2010) outlines the operational philosophies as follows:

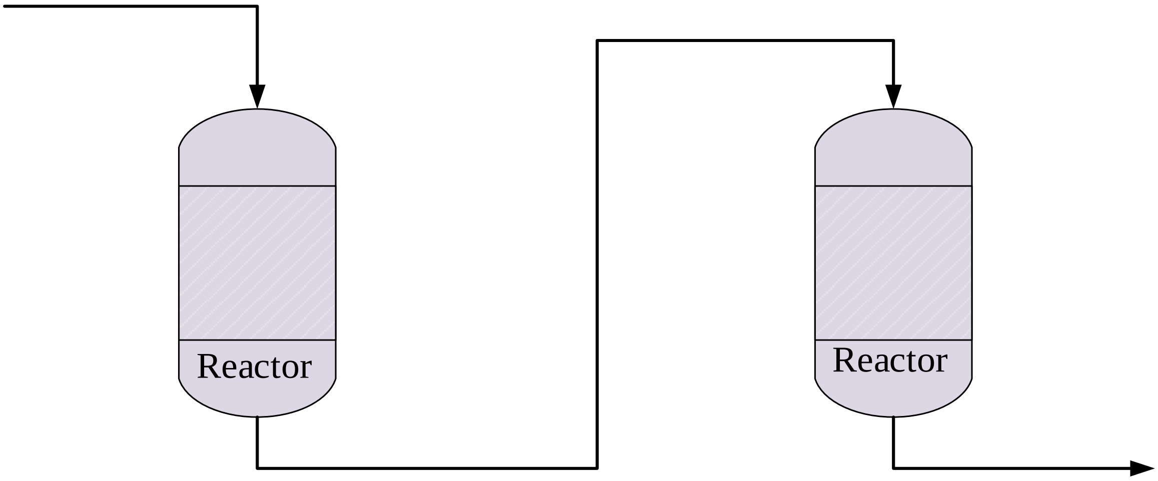


Figure 2.12: No intermediate storage

2.5.1. Finite intermediate storage (FIS) philosophy

This type of intermediate storage is characterized by the fact that the availability of storage is not guaranteed, which means that there might be a point in the process when the storage unit is filled to capacity and cannot be used for storage. FIS is useful when the completion time of one task does not coincide with the start of a subsequent task.

2.5.2. Unlimited intermediate storage (UIS) philosophy

Unlimited intermediate storage, unlike FIS, has unlimited storage availability as the name suggests. The UIS philosophy operates in a similar manner to FIS in that, the intermediate product is stored prior to processing in the next unit. The advantage of using UIS is that there are no constraints in terms of storage capacity and intermediate products can be stored immediately without any delays. This type of operational philosophy is used mostly in processes where the capacity of the storage unit far exceeds the capacity of the processing unit and is depicted in Figure 2.13.

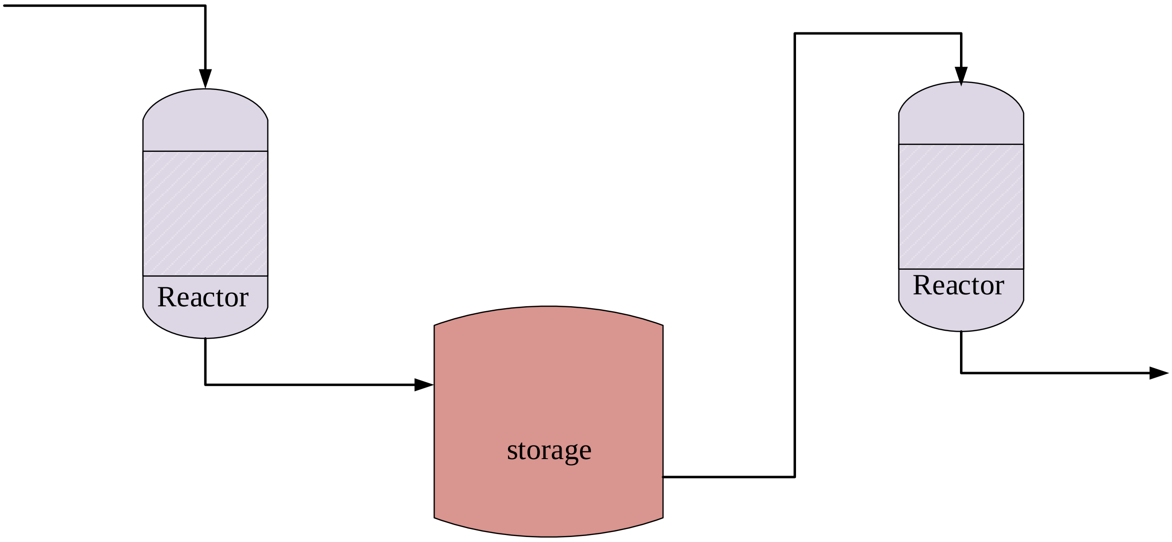


Figure 2.13: Unlimited intermediate storage

2.5.3. Common intermediate storage (CIS) philosophy

Common intermediate storage (CIS) operational philosophy makes use of a single storage unit for the storage of intermediate products from different processing units. This operational philosophy is normally applied when the products from each of the processing units are of the same nature but can also apply in cases where the products are different. It is important to ensure that there is no contamination of one product by the other. This can be achieved by thoroughly washing the storage unit prior to introducing the next intermediate product. The shortcoming of this type of operational philosophy is the cost of treating effluent. The CIS operation philosophy is shown in Figure 2.14.

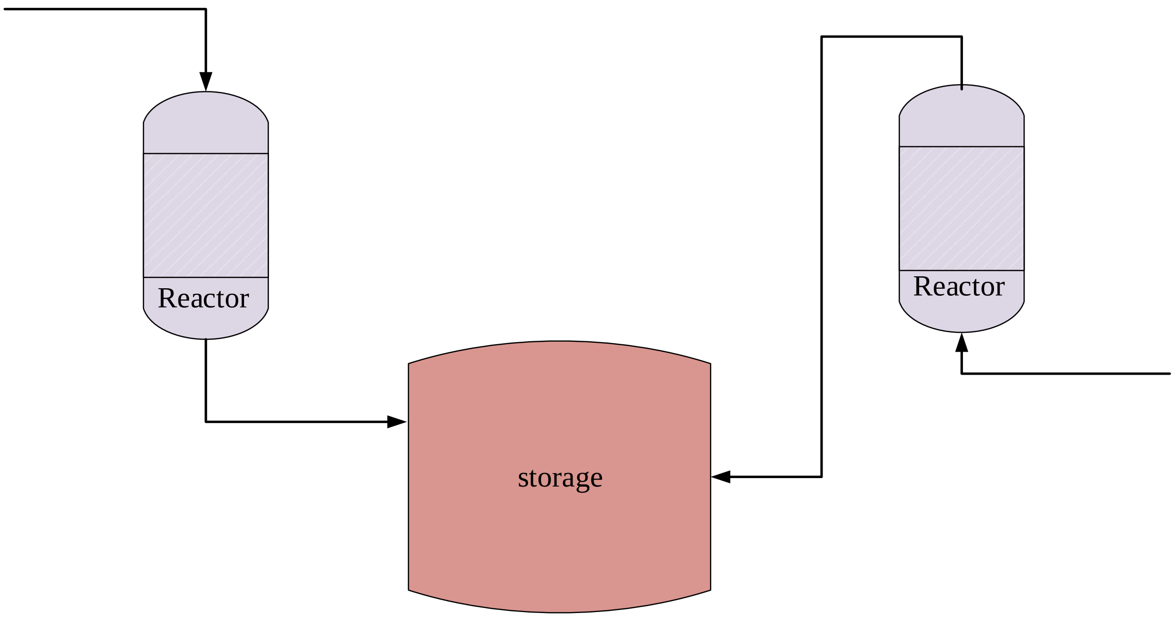


Figure 2.14: Common intermediate storage

2.5.4. Mixed intermediate storage (MIS) philosophy

In most batch plants in industry, processes are complex and require rigorous measures to ensure that the optimum processing conditions are achieved. This is normally done by applying a combination of the aforementioned operational philosophies, which is referred to as MIS operational philosophy.

2.5.5. Process intermediate storage (PIS) philosophy

This operational philosophy applies when the process units in the plant are used as storage units when the units are idle as depicted in Figure 2.15. This leads to benefits such as increased capital utilization of equipment as well as possible reduction in the size of the plant.

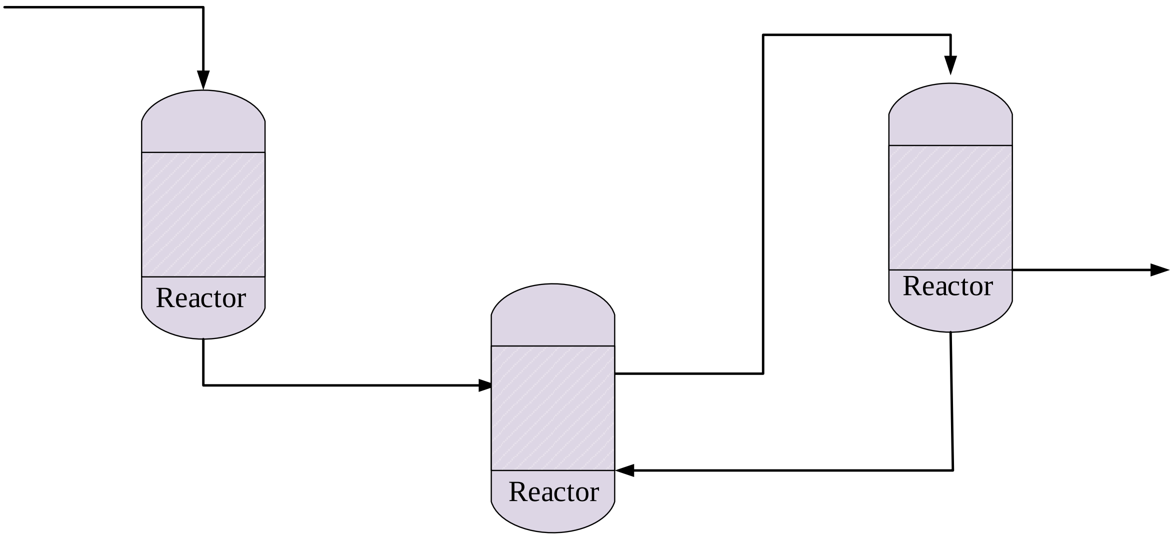


Figure 2.15: Process intermediate storage

2.5.6. Zero wait (ZW), Finite wait (FW) and Unlimited wait (UW) intermediate storage philosophy

The ZW, FW and UW intermediate storage operational philosophies are normally applied in processes where the stability of the product may fluctuate or vary throughout the process. In the instance where the product from a processing unit is unstable and needs to be processed immediately, the ZW operational philosophy is applied. The FW operational philosophy is applied when the product is only partially stable and can only be stored for specific time period before decomposition occurs. There are instances when the intermediate product is stable over a long period of time, and in such instances the UW operational philosophy is applied where the product is stored in either the processing unit itself or in a separate storage unit.

In order for the appropriate operational philosophy to be determined, an understanding of the process needs to be gained. This can be achieved through recipe representations, which include the quantity of material and sequence of the tasks to be performed.

2.6. Recipe representations

The representation of the recipe forms an important part of batch plants and it is a primary feature in the development of the mathematical technique since it aids in exploring the scheduling procedures of batch plants. There are different methods by which the recipe can be represented, these methods include the state task network (STN), the resource task network (RTN) and the state sequence network (SSN).

2.6.1. State task network (STN)

The state refers to the materials used or produced in the process in the form of raw materials, intermediates and the final products. The task refers to the unit operations that are performed in the equipment units. The state is illustrated as a circle and the task is illustrated as a rectangular box. An example of the STN representation is shown in Figure 2.16. The STN representation was proposed by Kondili et al. (1993).

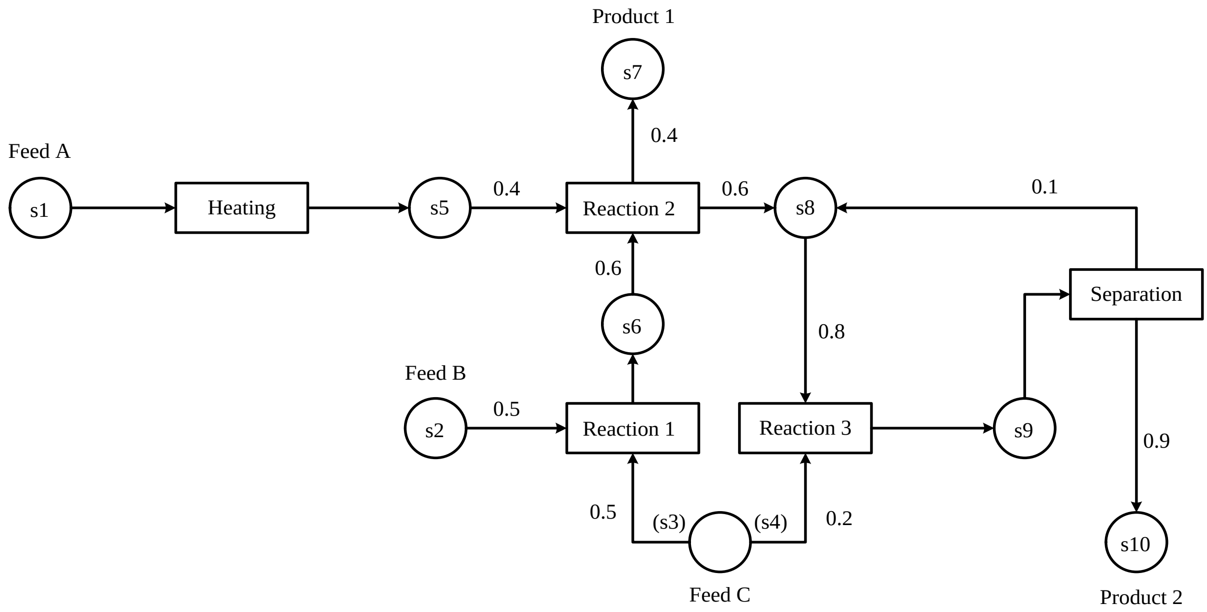


Figure 2.16: STN representation of a batch process (Kondili, et al., 1993).

2.6.2. Resource task network (RTN)

The STN was modified to form the RTN. The enhanced version refers to the resource node as raw materials, intermediates, products, and energy, manpower, storage and transportation facilities. The task node is, again, defined as unit operations that are performed in the equipment units together with transportation, cleaning and storage (Chen & Chang, 2009). The RTN representation was developed by Pantelides (1994). Figure 2.17 gives an illustrative example of the RTN.

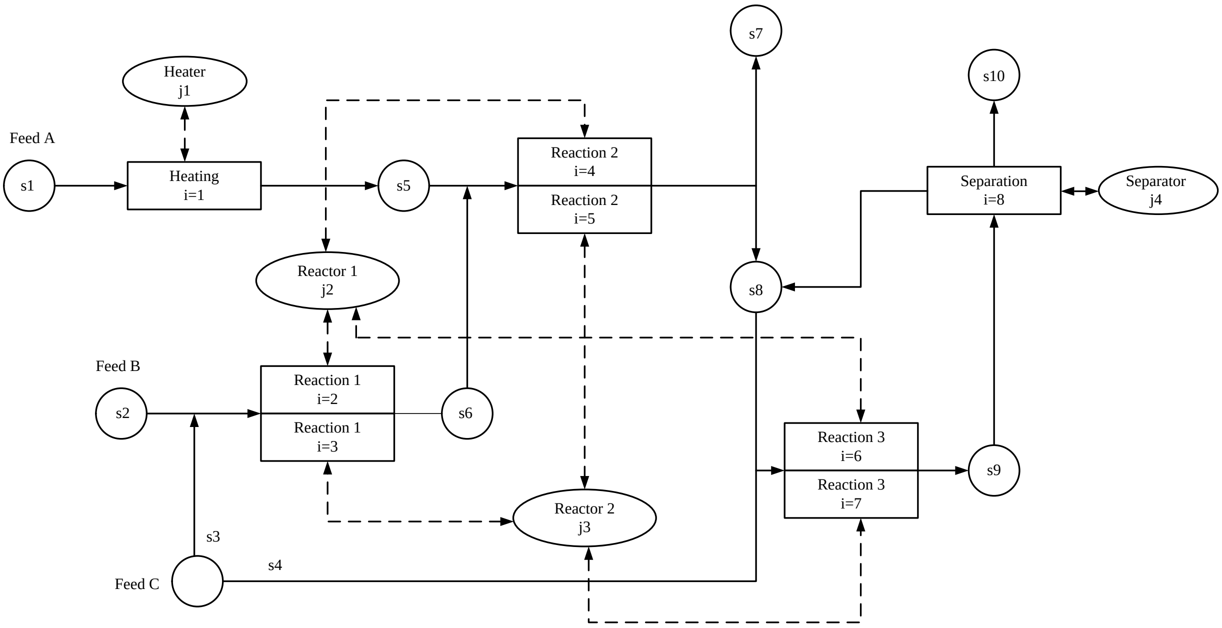


Figure 2.17: RTN representation of a batch process.

2.6.3. State sequence network (SSN)

The state sequence network proposed by Majozi and Zhu (2001) is similar to the state task network. The SSN differs in its replacement of tasks with sequences. The sequence node is defined as the point at which the state changes from one state to another in the process thus implying a process operation in a specific equipment unit. This is illustrated by the Figure 2.18.

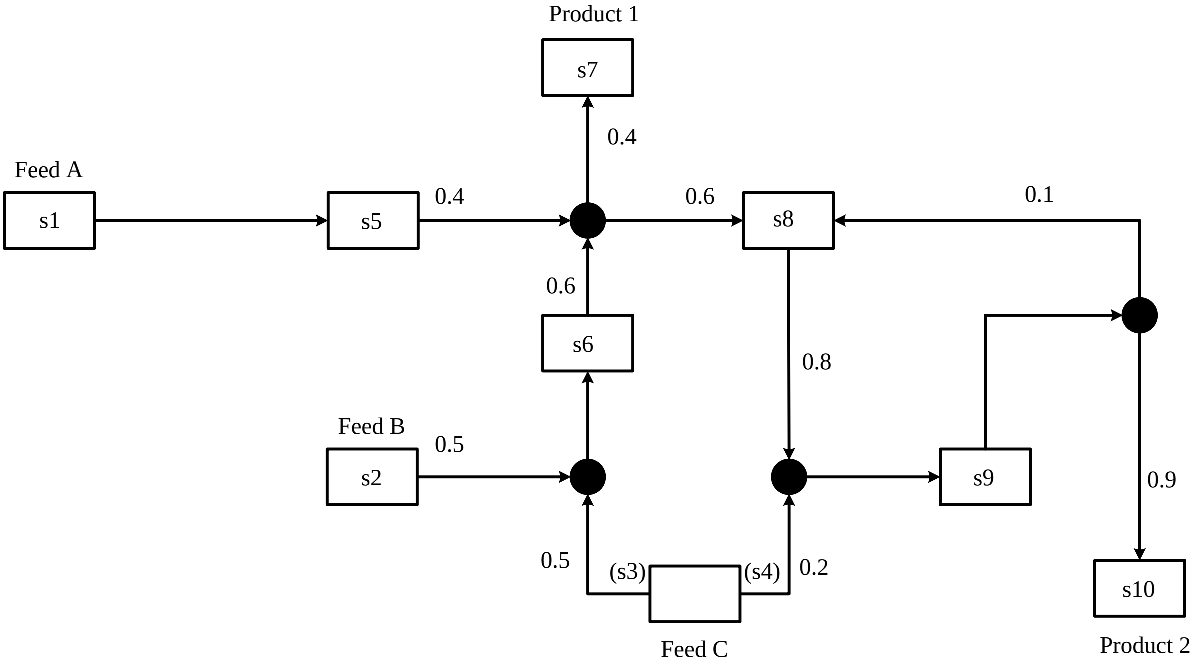


Figure 2.18: SSN representation of a batch process (Majozi, 2010)

2.7. Scheduling

Scheduling is required whenever there is competition for scarce resources among activities or tasks. A number of different products can be produced in one plant and thus it is important to determine a schedule for the plant in order to meet the order requirements of the different products. Scheduling, in this context, refers to the sequencing and the determination of the number of batches that will meet production requirements as well as the time associated with each batch throughout the time horizon. Castro et al. (2004) described scheduling as a decision-making process aiming to optimize one or more objectives by taking into account production requirements, available resources such as process units, materials and utilities, and their interactions in the process. Schedules can also be defined as fixed schedules that do not change or variable schedules that change depending in the process conditions. Scheduling has been mostly been categorised by the use of mixed integer linear programming (Pinto & Grossmann, 1994).

2.7.1. History of scheduling methods

There have been different types of methods used in batch plants in order to determine the optimised schedules of these processes. One such method was proposed by Suhami and Mah (1982) where the heuristic approach that resulted in a mixed integer nonlinear program (MINLP) was used in order to find the optimal design of multipurpose batch processes. This was achieved by randomly generating configurations and a set of rules of the process from which the optimal configuration was then chosen by using generalized reduced gradient code as the solver. This was an alternative to the branch and bound technique which sometimes results in tedious computational effort. The objective was to minimise the batch equipment cost of the plant. Heuristic methods, which can be less tedious than other methods, do not guarantee optimality.

Sanmarti et al. (1998) proposed a graphical formulation for multipurpose batch plants called S-graph. The formulation that was proposed used the schedule-graph as the basis of the representation and incorporated branch and bound algorithms for solving the problem effectively. The graph algorithm was used to evaluate the makespan which was then used as the lower bound in the branch and bound algorithm. The recipe of the products as depicted in Figure 2.19 is converted to a graphical representation of the recipe shown in Figure 2.20. The nodes on the graph in Figure 2.20 represent the production tasks and the arcs represent the precedence relationship among them. For a scenario where the number of batches is already known and the assignments of tasks to units is given, the sequence of tasks to be processed can be obtained and the sequence of tasks processed in a specific unit 1 can be outlined as task 1, 7 and 9 shown in Figure 2.21. The branch and bound procedure is given in Figure 2.22. NIS and UIS operational philosophies were taken into account in the formulation, because appropriate precedence relationships were chosen.

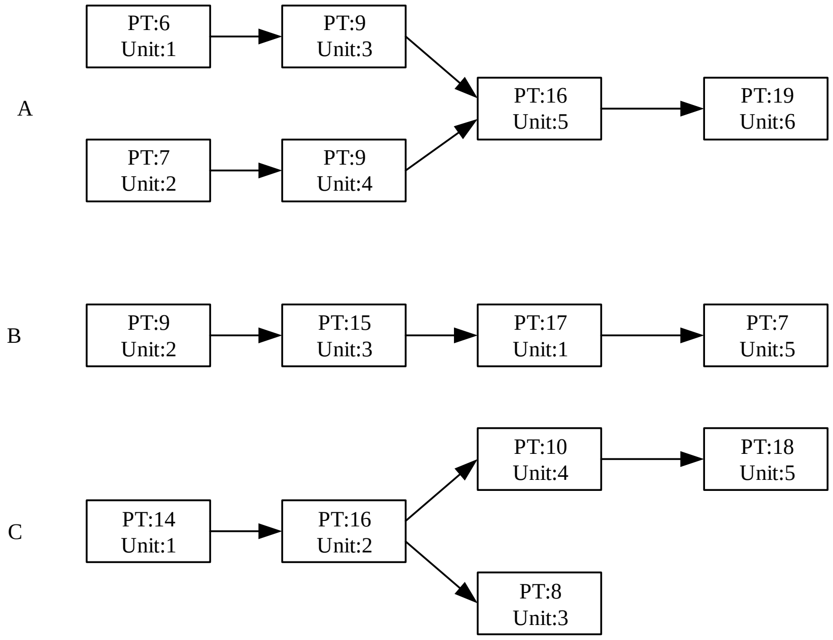


Figure 2.19: Recipe of the products produced in a batch process (Sanmarti, et al., 1998)

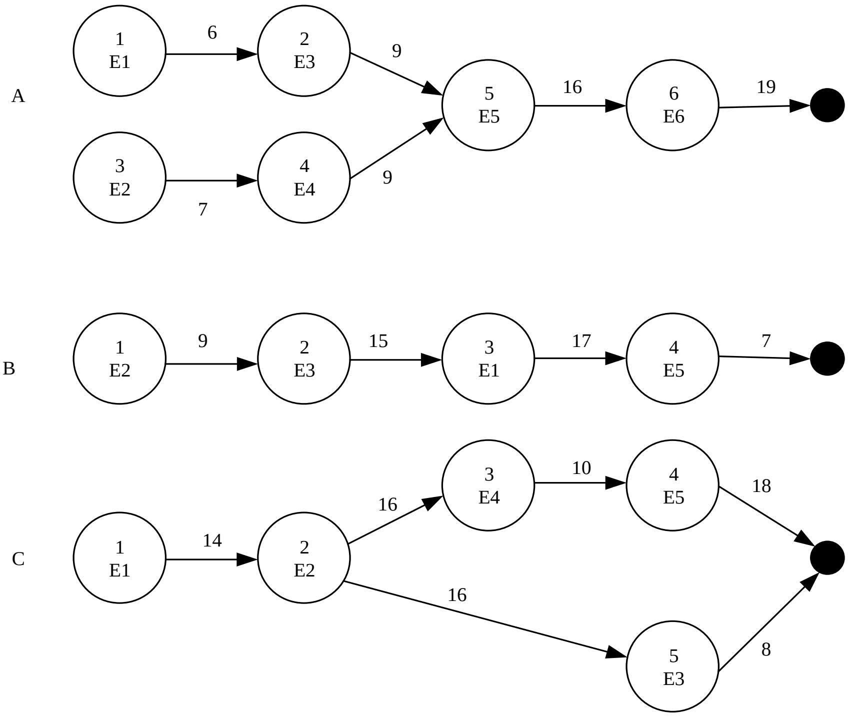


Figure 2.20: Graphical representation of the recipe produced in a batch process (Sanmarti, et al., 1998)

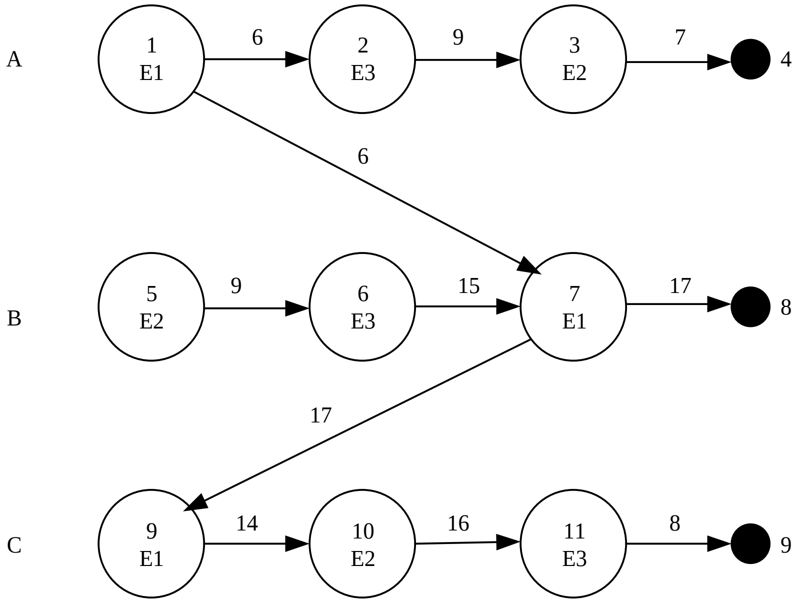


Figure 2.21: S-graph representation of a batch process recipe (Sanmarti, et al., 1998)

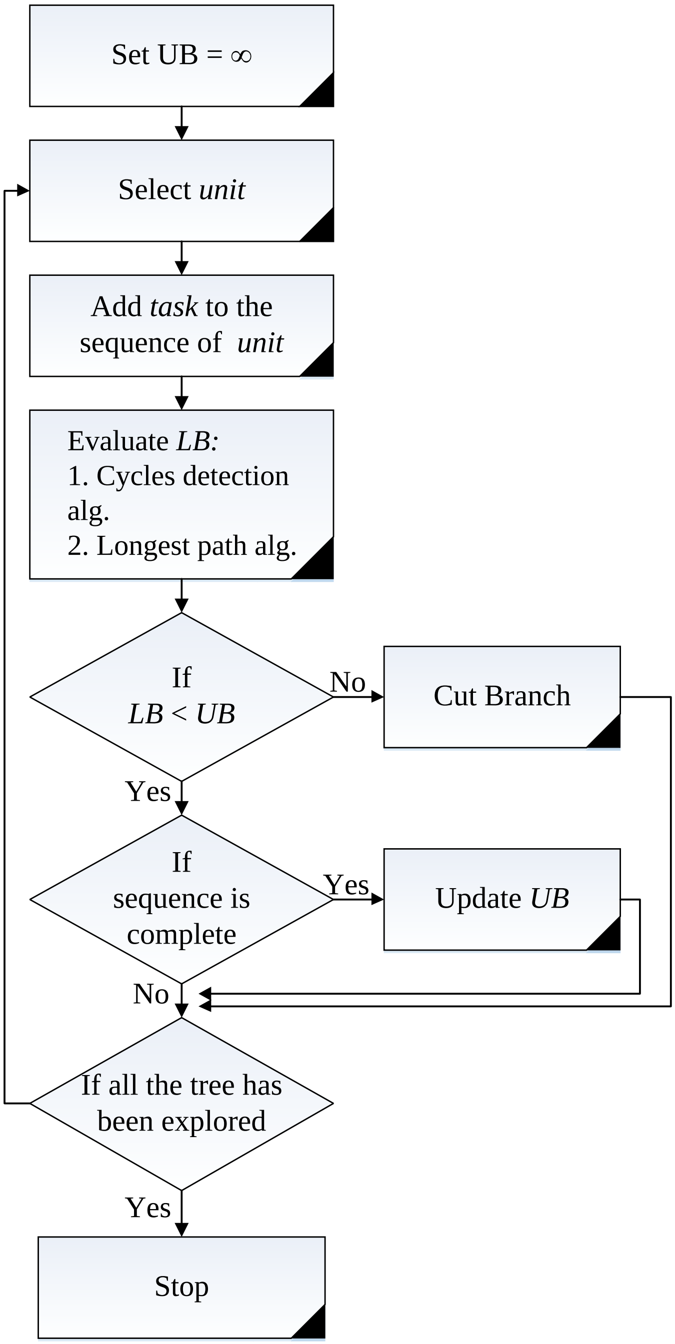


Figure 2.22: Branch and bound procedure used in solving mathematical formulations (Sanmarti, et al., 1998)

Other scheduling methods which use mathematical formulations based on different operational philosophies can also be used. Below are the different scheduling formulations based on the STN, RTN and SSN representations.

2.7.2. Scheduling methods using STN representations

Kondili et al. (1993) presented a scheduling formulation which used the STN. The formulation was based on an even discrete time representation and also took into consideration all types of intermediate storage policies. The following fundamental constraints needed to be satisfied;

- The resolution of conflicts when equipment items are allocated to tasks
- Limitations on the capacities of the units and storage stations; and
- Material balances

Batches of material were allowed to merge and spilt and the assignments of processing equipment to tasks were not determined a priori. The resulting MILP formulation led to a large number of binary variables and large CPU times which meant the formulation was computationally intensive.

The large computation requirement resulted in Shah et al. (1993) proposing a framework which detailed the computational issues of Kondili et al. (1993) formulation and the manner in which these computational issues can be overcome. The computational issue of the formulation proposed by Kondili et al. (1993) was due to the discrete representation of time being divided in a large number of equal intervals. Branch and bound procedure was used as the basic solution method. The branch and bound technique searches the entire search space and eliminates certain solutions by using previous estimates to obtain the optimal solution is (Shah, et al., 1993). Reformulation technique was applied to the allocation constraints where the integrality gap between the optimal solutions was considered. The integrality gap is the difference between the optimal solution and the relaxed solution. The aim was to decrease the integrality gap of the allocation constraints while all other things are left the same so that it can be proved that a smaller gap results in fewer branch and bound iterations. This was achieved by considering the way the constraints are structured. Reduction of linear programming relaxation, were applied to the model to reduce the size of the relaxed LP obtained after the reformulation techniques were applied to the allocation constraints. Post analysis of relaxed LP solutions was also done in order to reduce computational complexity.

Ierapetritou and Floudas (1998) introduced the continuous time formulation of short term scheduling by presenting the concept of event points. Event points are defined as the beginning or ending of a certain task with the specified time horizon. The concept of the formulation was that different binary variables defined the tasks and the units separately and resulted in a MILP formulation. However, this formulation resulted in a large number of variables in situations where processes involved many units.

Giannelos & Georgiadis (2002) proposed a formulation based on STN recipe representation and unit specific event-based time representation which resulted in a mixed integer linear programming model. The use of unit specific event-based time representation requires accurate depiction of the mass balances of states taking into account storage should the finite intermediate storage philosophy be deployed as well as sequence or timing constraints of tasks. The formulation proposed adequately takes into account the aforementioned. The timing constraints of states consumed by multiple tasks, states produced by multiple tasks and intermediate states are illustrated by Figures 23, 24 and 25. The constraints for states consumed by multiple tasks can be illustrated by figure which ensures that should a state be consumed by two tasks, the starting times of these tasks are the same for both tasks engaged in consuming the state. A similar argument is applicable for states produced by multiple tasks. The ending times of the two tasks producing a specific state must be the same. The duration constraint was adapted from the general size-dependent duration, constraint (1) to an inclusion of a buffer time duration constraint (2).

$$\theta_i = a_i + b_i B_i \tag{1}$$

$$\theta_i = a_i + b_i B_i + \theta_i^{buf} \tag{2}$$

Where a_i is the size-dependent contribution to the task duration and b_i is the term dependent on the batch size, B_i. The proposed formulation included θ_i^{buf} which is a relaxation term, buffer time.

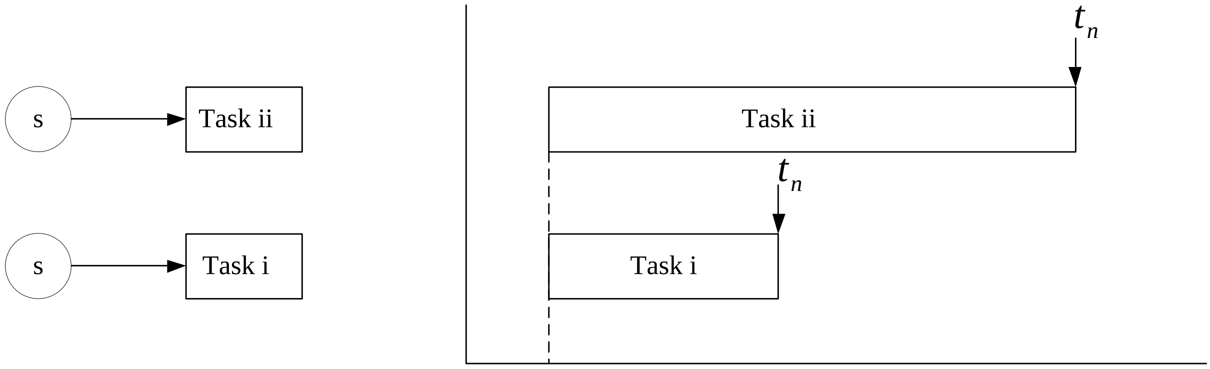


Figure 2.23: States consumed by multiple tasks (Giannelos & Georgiadis, 2002)

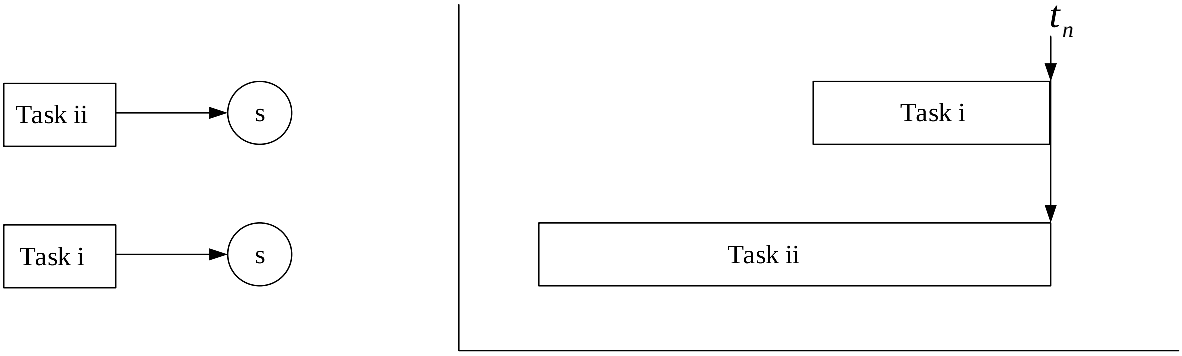


Figure 2.24: States produced by multiple tasks (Giannelos & Georgiadis, 2002)

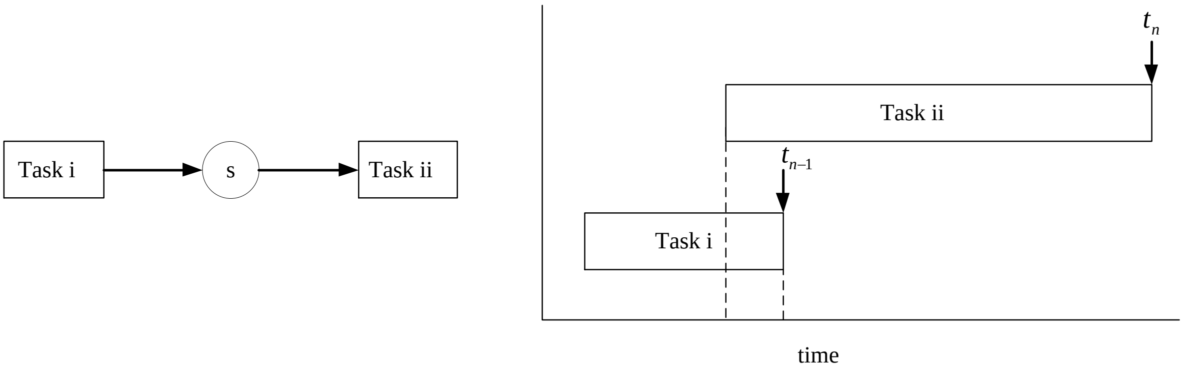


Figure 2.25: Intermediate state (Giannelos & Georgiadis, 2002)

A global event-based continuous time model was proposed by Maravelias and Grossmann (2003). The STN recipe representation was employed in this formulation and included accounting resource constraint, variable batch sizes and processing times, various storage policies such as UIS, FIS, NIS and ZW, batch mixing/splitting and sequence-dependent changeover times. Maravelias and Grossmann (2003) stated that the key features of the formulation included assignment constraints expressed using binary variable that are only defined for tasks and not for units. The time matching constraints were only applicable for the finishing times of the tasks and not for the starting times. A new class of inequalities was introduced which improved the LP relaxation and resulted in a faster model.

2.7.3. Scheduling methods using RTN representations

The concept of resource task network was extended by Zhang and Sargent (1996) by proposing a unified mathematical formulation which is used to determine the optimal operating conditions of a mixed production facility consisting of multipurpose batch processes. The aim of their contribution was to model the mixed production facility by performing tasks which change certain resources into other sets of resources. The mathematical formulation for the multipurpose batch process was in the form of a MILP formulation.

Schilling and Pantelides (1996) presented a scheduling formulation based on the RTN which used the continuous representation of time. The continuous representation of time was chosen because of the large number of intervals which had to be used in the discretization time formulation in order for a certain degree of accuracy to be maintained for the schedule. Although the continuous formulation resulted in a smaller number of intervals, the formulation also resulted in a large integrality gap and rendered the solution obtained using standard branch and bound highly problematic. Schilling and Pantelides (1996) proposed a novel branch and bound algorithm that branches off both binary and continuous variables in order to decrease the integrality gap.

Castro et al. (2001) presented a formulation which was based on RTN and global-event based time model. The formulation was based on that of Shilling (1997) which resulted in a mixed integer non-linear programming model. The formulation was then linearized to a mixed integer linear programming model. The model presented by Shilling (1997) was difficult to solve due to the time constraints which were introduced. Castro et al. presented a formulation were the time constraints used by Shilling (1997) were relaxed to give a more flexible constraint by changing the “equal to” sign to the “greater or equal to” sign for the processing time as shown below. Constraint (3) was adapted to constraint (4),

$$T_{t'} - T_t = \alpha_i \bar{N}_{i,t,t'} + \beta_i \xi_{i,t,t'} \qquad (3)$$

$$T_{t'} - T_t \geq \alpha_i \bar{N}_{i,t,t'} + \beta_i \xi_{i,t,t'} \tag{4}$$

Where T_t is the absolute time of event point *t*, α_i is the size-dependent term in the processing time of task *i*, $\bar{N}_{i,t,t'}$ is the binary variable that assigns the end of task *i* which began at time *t* to point *t'*, β_i is the size-dependent term in the processing time of task *i* (time required to process one unit of material) and $\xi_{i,t,t'}$ is the total amount of material processed by the instance of task *i* starting at event point t and finishing at event point *t'*.

The model introduced the concept of the allowing, if possible, finite storage within the processing equipment of the involved raw materials and/or products. This methodology can decrease the number of event points that are used in the model which is important for the efficiency of the solver. The model resulted in less CPU time compared to the model by Shilling (1997) as it was easier to solve due to the relaxation. The formulation also explores degeneracy exhibited by the problems where the presented formulation resulted in a lower degree of degeneracy as compared to model proposed by Shilling (1997).

Castro et al. (2004) used the mathematical formulation of Castro (2001) as a basis for the proposed formulation by extending it to both batch and continuous processes. The model was based on RTN recipe representation and the global event-based time representation. The main differences between the models was that the proposed one uses a more efficient set of constraints for batch tasks subject to zero-wait policies and uses a different set of timing constraints that improved linear relaxations of the model thus having a profound effect on the computational cost. A number of assumptions were made in order to reduce the complexity of the mathematical formulation. The first assumption made was to ensure that all equipment resources, with the exception of storage tanks, are considered individually. This means that should there be two or more identical pieces that exist, one resource will need to be defined for each item. The other assumption made was to ensure that only one task can be executed in any given equipment resource at a certain time. The mathematical formulation resulted in a simpler model for short-term scheduling which was evident when the proposed model was compared to other short-term scheduling models.

A mathematical model was presented by Shaik & Floudas (2008) which was based on RTN formulation using unit specific event-based time model. the formulation included unlimited as well as finite storage for different intermediate states. Finite storage was taken into account without considering storage as a separate task but rather, was included within the production tasks. The mathematical formulation was aimed at maximising profit which was defined as the amount of product produced multiplied by the selling price. Another objective function which was considered was the minimisation of the makespan for a certain amount of product produced. The cconstraints which were taken into account included excessive resource balances, capacity, sequencing and storage constraints. Additional tightening constraints were included in order for all tasks to occur within the given time horizon so that the time search space is minimised.

2.7.4. Scheduling methods using SSN representations

In order to develop a typical short term scheduling mathematical model, Majozi and Zhu (2001) presented a formulation in which the SSN representation is used to model a batch process. The model was aimed at determining the optimal schedule for tasks within the time horizon of interest, the amount of material processed in each unit and the amount delivered to customers over the entire time horizon. The formulation made use of time points as presented by Schilling and Pantelides (1996) distributed over the time horizon of interest. The binary variables used in the formulation correspond to the states i.e. *y(s,p)*. The mathematical model applied to the literature example consisted of defined sets, variables, parameters, capacity and duration constraints, material balances, sequence and assignment constraints and storage constraints. The following information was given:

- The production recipe for each product including mean processing times for each operation
- The available unit and their capacities
- The maximum storage capacity for each material
- The time horizon

It was required to determine:

- The optimal schedule for the tasks within the time horizon
- The amount of material processes in each unit at any particular point in time within the time horizon
- The amount delivered to customers

The formulation used uneven time discretization with state to state correspondence and resulted in less binary variables compared to other time formulations and yielded a faster CPU time.

Seid and Majozi (2012) proposed a mathematical formulation, based on the SSN representation, which was categorised in two separate models named ML1 and ML2. The difference between the two models is that ML1 did not take into account the nonsimultaneous transfer of material, which is advantageous in allowing for the flexibility of time in the time horizon. It is important that when the case study in question is of a finite intermediate storage nature, the model represents it accordingly. In this formulation, Seid and Majozi (2012) took into account the constraints for the FIS accurately.

The mathematical formulation proposed by Seid and Majozi (2012) comprises of allocation, capacity, material balance, duration, sequence, storage, time horizon and tightening constraints which are described by the given sets, variables and parameters. A summary of the model proposed by Seid and Majozi (2012) is detailed below.

Sets

S	$\{s \mid s$ any state$\}$
$s_{in,j}^{sc}$	$\{s_{in,j}^{sc} \mid s_{in,j}^{sc}$ any consumed state$\}$
$s_{in,j}^{sp}$	$\{s_{in,j}^{sp} \mid s_{in,j}^{sp}$ any produced state$\}$
s^{p}	$\{s^{p} \mid s^{p}$ any product$\}$
p	$\{p \mid p$ time point$\}$

Variables

$t_u(s_{in,j}, p)$	Starting time of a task
$t_p(s_{in,j}, p)$	Finishing time of a task
$mu(s_{in,j}, p)$	Amount of material processed
$qs(s_{in,j}, p)$	Amount of stated stored
$t(j, p)$	Binary variable for usage of state produced by unit j at time point p
$x(s, p)$	Binary variable for availability of storage for state s

Parameters

H	Time horizon
$\tau\left(s_{in,j}\right)$	Coefficient of constant term of processing time of task
$\beta\left(s_{in,j}\right)$	Coefficient of variable term of processing time of task
$\rho^{sc}_{s_{in,j}}$	fraction of state s consumed
$\rho^{sp}_{s_{in,j}}$	Fraction of state s produced

The allocation constraints are used to allocate a task to a specific unit at a specific point in time. The capacity constraints are necessary in batch processes due to the limitation of the capacity of the units on the batch size. In order for the batch size to be determined, the capacities of all units must be taken into account. The mass balance states that the mass of each state stored at time point *p* must be equal to the mass stored at the previous time point and any mass produced at the previous time point. Any mass that has been used in the current time point must be deducted from the mass stored. Constraint (5) describes the mass balance.

$$qs(s,p) = qs(s,p-1) - \sum_{s_{in,j} \in S^{sc}_{in,j}} \rho^{sc}_{s_{in,j}} mu\left(s_{in,j},p\right) + \sum_{s_{in,j} \in S^{sp}_{in,j}} \rho^{sp}_{s_{in,j}} mu\left(s_{in,j},p-1\right) \qquad (5)$$

As mentioned previously, time is an important factor in batch processes and therefore the duration of a task in specific unit must be considered and addressed. Constraint (6) describes the duration of the tasks which states that the time at which a task ends is equal or greater than the time at which the task starts plus he processing time.

$$t_p\left(s_{in,j},p\right) \geq t_u\left(s_{in,j},p\right) + \tau\left(s_{in,j}\right) y\left(s_{in,j},p\right) + \beta\left(s_{in,j}\right) mu\left(s_{in,j},p\right) \qquad (6)$$

These constraints were used to accurately take into account the finite intermediate storage philosophy. In previous models, these constraints were overlooked hence resulted in sub-optimal results and the final schedule resulted in the unlimited intermediate storage philosophy.

The sequence constraints are divided into same task in same unit, different task in same unit, different tasks in different units and sequence constraints for FIS policy. Constraint (7) states that the amount of state *s* used can either come from storage or from other units that produced state *s*. Constraint (8) then states that 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,

$$\sum_{s_{in,j} \in S_{in,j}{}^{sp}} \rho^{sc}_{s_{in,j}} mu\left(s_{in,j}, p\right) \leq qs\left(s, p-1\right) + \sum_{s_{in,j} \in S^{sp}_{in,j}} \rho^{sp}_{s_{in,j}} mu\left(s_{in,j}, p-1\right) t\left(j, p\right) \tag{7}$$

$$t_p\left(s_{in,j'}, p-1\right) \leq t_p\left(s_{in,j}, p-1\right) + H\left(2 - y\left(s_{in,j'}, p\right) - y\left(s_{in,j}, p-1\right)\right) + H\left(x\left(s, p\right)\right) \tag{8}$$

Additional storage constraints were included in the model that make sure the amount of product or intermediate stored at a point in time does not exceed the capacity of the available storage vessels. Time horizon constraints ensure that all tasks take place within the given time horizon and tightening constraints state that the usage and production of all states should be in within the time horizon.

The objective function of the mathematical formulation was given as either the maximisation of the amount of product produced or the minimisation of the makespan of the process as described by constraints (9) and (10), respectively.

$$\max \sum_{s} price\left(s^p\right) qs\left(s^p, p\right) \tag{9}$$

Or

$$\min H \tag{10}$$

Scheduling techniques are incorporated to heat integration techniques in order for the energy consumption in batch plants to be minimized.

2.8. Heat integration

Certain industries that manufacture products using batch processes, such as brewing and dairy are as energy intensive as continuous processes and as such energy minimisation in batch processes has been an area of interest in research. Just as in continuous processes, there exists an opportunity for heat integration in batch processes in the form of direct and indirect heat integration. Direct heat integration is when two streams or tasks, one that requires heating and another that requires cooling exchange heat with one another. In order for heat exchange to happen, the tasks must occur at the same or similar time. Indirect integration is the use of a heat transfer medium (HTM) in a heat storage vessel that is used to heat or cool a stream or task according its energy requirements. Indirect heat integration is introduced due to its ability to create flexibility in the plant because of the time limitations that exist in batch plants.

Heat integration in batch processes can be achieved through pinch analysis (graphical techniques), mathematical modelling and in some instances the use of heuristics. Heat integration first started being published in the 80s of the 20th century by Linhoff (1988) who introduced the concept of developing the Pinch Technology for the synthesis of Heat Exchanger Networks (HENS). This type of heat integration has extensively been researched for continuous processes but could not be directly applied to batch processes due to the intrinsic time characteristic of these processes. Research has since been done on heat integration in batch plants by applying pinch analysis with predetermined schedules and using mathematical models to simultaneously optimise schedules and heat consumption. Mathematical models have also been used with predetermined schedules to optimise energy. A hybrid of pinch analysis, mathematically modelling and heuristics has also been applied to minimise energy in batch processes.   .

2.8.1. Graphical techniques

Energy minimisation in batch plants was first conducted through the use of graphical techniques. There are two main methods which are used in the graphical techniques, which is the time average model as well as the time slice model. The time average model was first introduced by Clayton (1986) where the energy of each stream was averaged over the batch cycle time. The minimum external utility requirement is then determined by taking into account the heat exchanged internally between streams. This method does not consider the discontinuous existence of streams which results in an overestimation of energy exchanged between streams.

Time slice model uses the schedule of the batch process and divides the starting and ending times of tasks into slices or intervals. Each interval is then observed as a continuous process. The pinch point of every interval is then obtained in a similar manner like that in continuous processes. This method was first introduced by Obeng and Ashton (1988).

Wang and Smith (1995) proposed a formulation for energy and water minimisation based on time pinch analysis. Heat integration was achieved through the pinch analysis technique, where due to the nature of batch processes, time was treated as a primary constraint and temperature as a secondary constraint. Shifting of stream temperatures was implemented by decreasing the supply and target temperatures of the hot streams by half the minimum allowable temperature difference while the supply and target temperatures of the cold streams were increased by half the minimum allowable temperature difference. The supply and target temperatures were separated into different intervals and pinch analysis was implemented by first considering the time at which the batches occurred.

The methodology presented by Yang, et al. (2014) was based on the methodology proposed by Liu et al. (2011) which used the Pseudo-T-H diagram (PTHDA) and the time slice model. The model applied both direct and indirect heat integration with the objective of minimising the total annual cost (TAC). The initial and target temperatures of streams were known before hand as well as the starting and ending time of the streams. The capacity flow rate of each stream was given as a parameter. The indirect integration operation, shown in Figure 2.26, used two heat storage vessels, one with a hot medium fluid maintained at a higher temperature and the other with a cold medium fluid maintained at a lower temperature. The hot heat storage vessel was then used to heat up a cold stream while the cold heat storage vessel was used to cool down a hot stream. External utilities can also be used in order to assist in reaching the target temperatures of the respective streams, shown in Figure 2.27. The method used to synthesize the batch HEN with heat storage vessels was done graphically by the pinch methodology which is only limited to two time intervals. The pinch point is used to determine where to place the heat storage vessels. The initial temperatures of the two heat storage vessels were also determined through an iterative process.

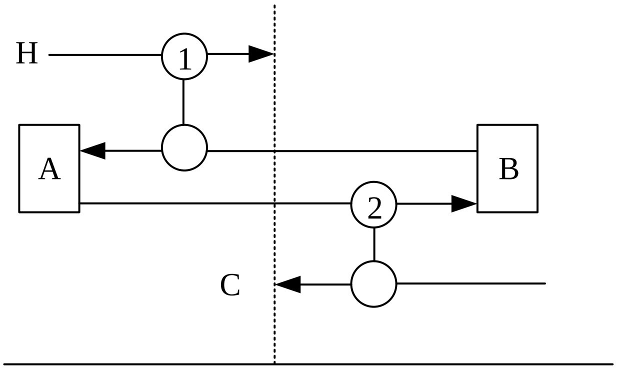


Figure 2.26: Indirect heat integration operation (Yang, et al., 2014)

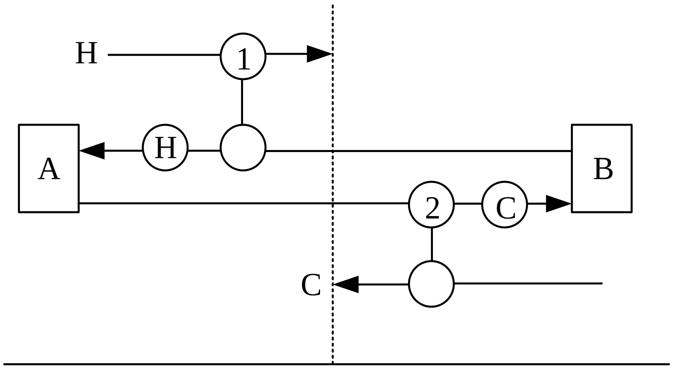


Figure 2.27: Indirect heat integration with utilities (Yang, et al., 2014)

Chaturvedi & Bandyopadhyay (2014) proposed a methodology where pinch analysis was used to find the minimum utility requirements of a batch process with a fixed schedule. The proposed method was aimed at overcoming the limitations that occured when using Time – Dependent Heat Cascade Analysis (TDHCA). The detailed designs of the heat exchangers, heat storage vessels, piping, etc. were not taken into account in the formulation and indirect heat integration was used between intervals by using a heat fluid intermediate. The minimum energy requirement was calculated using Problem Table Algorithm (PTA) or Modified PTA (MPTA) and Grand Composite Curves (GCC), Modified Grand Composite Curves (MGCC) and Time-Level Grand Composite Curves (TGCC). The flow diagram for the proposed formulation is shown in Figure 2.28. This method can be applied to single batch processes as well as cyclic batch processes.

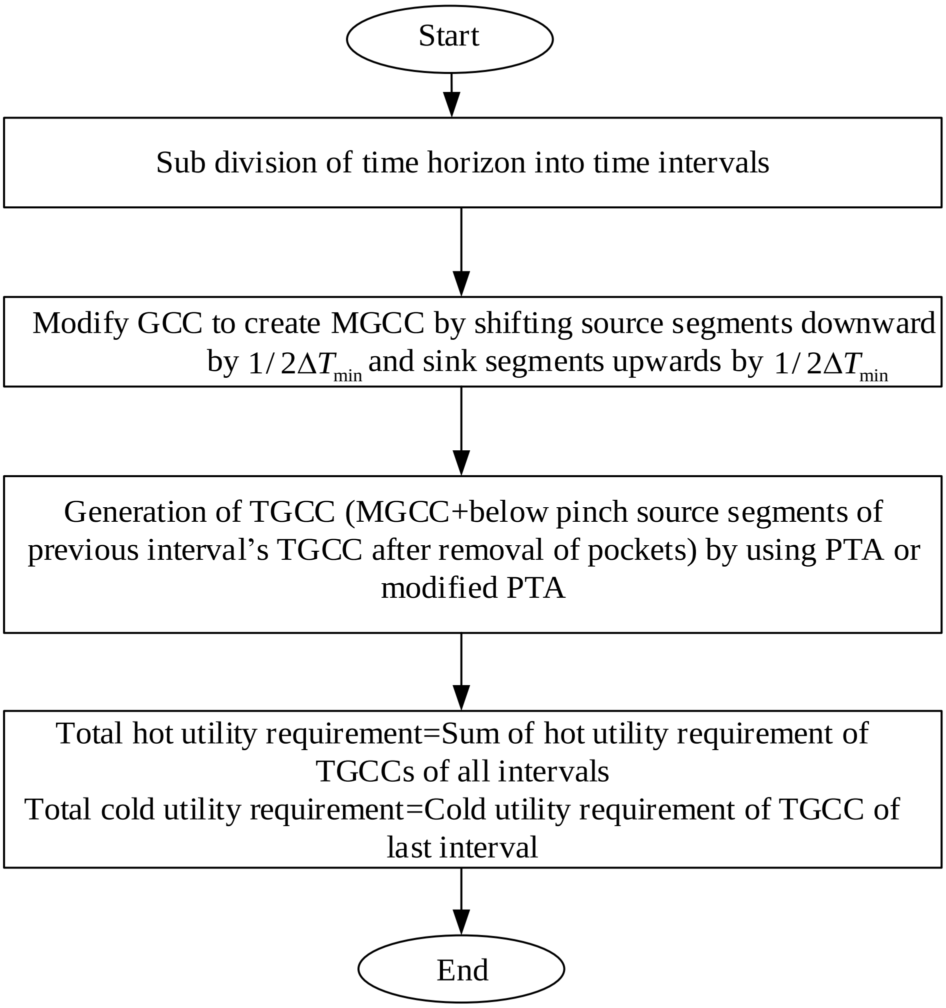


Figure 2.28: Flow diagram for energy targets (Chaturvedi & Bandyopadhyay, 2014)

The novelty of this paper presented by Chaturvedi, et al. (2016) is the shifting or delaying of product streams, in order for the product streams to be integrated with available cold/hot stream, later in the time horizon. A fixed schedule was used with cold and hot streams having predetermined starting and finishing times. The principles of pinch technology were applied by using the grand composite curve categorized as product grand composite curve and intermediate grand composite curve, to determine the cold and hot utility targets. The paper also took into account direct and indirect heat integration where direct integration was achieved through product streams being delayed or shifted to later intervals and product streams exchanging heat with intermediate streams in one interval. Indirect heat integration was obtained through an intermediate heat transfer fluid which can be used in later intervals.

Although graphical techniques offer conceptual insight, the techniques have proved to be insufficient due to their use of time as a parameter, which implies that the start and ending times are specified a priori. In order to obtain a more realistic representation of batch processes, time should be allowed to vary, and this can be achieved through mathematical modelling techniques.

2.8.2. Mathematical techniques

Time can be captured in its exact form through the use of mathematical modelling as demonstrated by Ivanov et al. (1992). The work done by Ivanov et al. (1992) was aimed at designing a heat exchanger network that pairs batch vessels, resulting in the minimization of total cost, when a fixed schedule is used. In the study, Ivanov et al. (1992) proposed a method which combines heat integration and temperature correction by the use of external heating and/or cooling agents. The utilization of heat in batch processes was achieved through process integration. However, in practice, the desired final temperature is not reached simultaneously and this warrants additional heating and/or cooling in order to correct the temperature. This is achieved through the use of an external subsystem in which external heating or cooling agents are used. In the formulation, Ivanov et al. (1992) developed a method of heating and cooling which combined heat integration and temperature correction simultaneously in time.

Papageourgiou et al. (1994) argued that the problem of scheduling in batch plants should, above cost of utilities and raw materials, include heat integration as an integral part in maximizing production over a given time horizon. The study conducted by Papageourgiou et al. (1994) involved both direct and indirect heat integration in batch plants. In the formulation, indirect heat integration made use of a heat transfer medium (HTM). It was assumed that the HTM was available at a number of different temperature levels, and was stored in a separate, well-mixed and insulated storage tank. The HTM provides some degree of flexibility when it comes to the timing of the operations that need to be either cooled or heated. However, the storage of energy can only be achieved over a limited period of time due to heat losses to the environment. The study presented a mathematical formulation that incorporated heat integration with the mathematical formulation presented by Kondili et al. (1993) for the short-term scheduling of multipurpose batch plants using even time discretization (discrete time representation). The formulation was aimed at selecting an optimum schedule that maximises process economics with due regard taken for the value of the products and the cost of raw materials and utilities. Although this heat integration method determines the optimum schedule, due to the even time discretization, it has many binary variables.

Bozan et al. (2001) presented a study in which scheduling as well as utility usage was considered. An integrated approach was developed which first synthesised the campaign set of the batch process through a simple algorithm. Once the campaign set was determined, heat exchange opportunities were explored through the placement of heat exchangers. The sizes of the heat exchangers were obtained through a nonlinear mathematical model. The parameters obtained through the campaign determination and the heat exchangers placement were used as input data for a mixed integer nonlinear programming model formulation which optimises the heat exchanger network of the process. The objective of the formulation was to minimise the cost of energy consumption.

Barbosa-Povoa et al. (2001) presented a study that was aimed at designing a batch process plant which considered the operation of the plant as well as the energy requirements. The formulation resulted in a mixed integer linear program which was able to dictate the main processing equipment required, the storage vessels, interconnections as well as the auxiliary equipment required for direct heat integration to take place. The model also allowed for different types of heat transfer equipment to be considered such as heat exchangers and serpentines. The formulation was based on the work of Barbosa-Povoa and Macchietto (1994) which considered the design of multipurpose batch plants without the utility considerations.

It is beneficial to ensure the formulation of a mathematical model for heat integration is built on an optimum process schedule and the time dependence of batch plants is taken into account accordingly. This was achieved by the formulation presented by Majozi (2006). In the formulation, an extension of the scheduling model proposed by Majozi and Zhu (2001), based on a continuous time framework and SSN representation, was used. The objective was to determine the production schedule associated with maximizing heat transfer and profit. The profit was defined as the difference between revenue and the utility costs. An assumption made in the formulation was that there was sufficient temperature driving force between matched tasks for process-process heat transfer. Where heat integration could not supply sufficient heat, external utilities were used to compensate for the deficit (Majozi, 2006). The mathematical formulation consisted of sets, variables, Glover transformation variables, parameters and equations. Glover transformation (Glover, 1975) was used to linearise the bilinear terms that arise in the mathematical formulation in order to yield an overall formulation that guarantees a global optimum. The mathematical model that was formulated consisted of a complete MILP formulation for direct heat integration.

Behdani et al. (2007) proposed a formulation that was aimed at extending the scheduling formulation and incorporating utilities associated with different tasks in the plant. The formulation presented in the paper separates the scheduling and the utility models. The scheduling model used the state task network recipe representations and the unit specific event based continuous time representation. The model was for facilities comprising of both batch and continuous operations. It is important to note that the concept of instantaneous utility consumption/production management was applied to the formulation. The utility constraints were categorized as consumption, availability and supply constraints while focusing on steam, cooling water and electrical energy as utilities. The objective function was input as a multi-objective function which was a cost function that included revenue, utility cost, switching cost and fluctuation penalty.

Chen and Ciou (2008) presented a study that took only indirect heat integration into account. The possibility of direct heat integration was not taken into consideration due to the fact that a predetermined schedule of the process was used which only considered the production of one overall batch, meaning each task only occurred once in the time horizon. An inherent characteristic of the mathematical formulation was that there should be a minimum of two heat storage tanks in the process. This was because the HTM from a certain tank absorbed heat from a hot unit then was sent to a storage tank until a time at which the HTM would reject the heat to a cold unit, thereafter return to the initial tank. It is evident that the proposed formulation is more suited for the application of indirect heat integration in multiproduct batch plants instead of multipurpose batch plants.

The formulation by Chen and Ciou (2008) did not determine the number of storage tanks but rather stipulated it as a parameter. The model was applied to two case studies. The first case study was compared to a pinch analysis adaptation of indirect heat integration. The proposed mathematical formulation yielded better results in the minimisation of the external utility consumption compared to the pinch analysis adaptation approach. A more complex case study was also presented, in which indirect heat integration with two and three storage tanks was analysed.

Halim and Srinivasan (2008) proposed a formulation that was aimed at minimising the utility consumption in batch processes while simultaneously optimising the scheduling. This was obtained through the use of a multi-objective function. The first part of the model was the optimisation of the schedule through slot-based continuous time formulation. The objective was to minimise the makespan of the plant. Heat integration opportunities were explored based on the solution obtained from the schedule. The solution from the scheduling model and the heat integration model were then used to obtain the Pareto solutions set.

A model aiming at incorporating direct heat integration through the basis of resource task network scheduling was presented by Chen and Chang (2009). The scheduling and the integration were carried out simultaneously and both short term scheduling and periodic scheduling were taken into account. The RTN recipe representation is seen to be inclusive of the tasks that occur in batch operations from a holistic point of view and that is the reason the formulation was based on RTN. The heat integration part of the model was a more general form of an adaptation of the model proposed by Majozi (2006).

Majozi (2009) extended the direct heat integration based SSN proposed by Majozi (2006) by including indirect heat integration. The formulation was presented in the form of a mixed integer linear program. The main advantage of this mathematical formulation is that the start and end times of the processes need not be known before modelling the formulation. This type of formulation also requires very few binary variables because the continuous time model is used. The mathematical formulation was used on a case study, in which production scheduling data, duties for tasks, cost of utilities, operating temperatures, minimum allowed temperature differences and the available heat storage capacity were given. It was also assumed that there were sufficient temperature driving forces between the tasks for process-process heat transfer. The formulation performed on the case study showed that less energy, in terms of cost of external utilities, is required when direct heat integration is applied and even less energy is required when indirect heat integration is considered.

Stamp and Majozi (2011) aimed to surpass previously encountered challenges such as using predetermined production schedules and using methods based on either direct or indirect heat integration by optimising the schedule together with the direct and indirect heat integration. The optimisation of the size and initial temperature of the heat storage vessel was also considered. The objective was to maximise profit through the minimisation of external energy consumption. Heat losses of the storage vessel were taken into account in the mathematical formulation which had previously not been done by Majozi (2009). Figure 2.29 shows the design of the heat storage vessel. The mathematical model was used on a literature example, a multipurpose batch facility, and on an industrial example. The results showed that using the proposed mathematical formulation results in a higher performance index (revenue-utility costs) than when no heat integration is applied to the example or when only direct heat integration is applied to the example. The optimum capacity of the storage medium was obtained, as well as the optimum initial temperature of the storage medium.

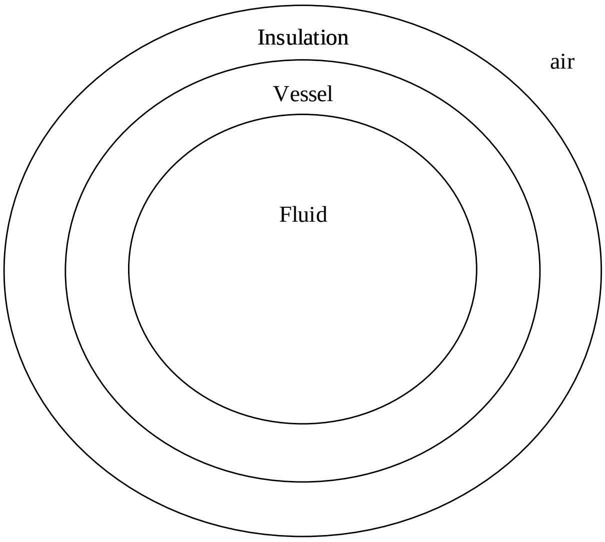


Figure 2.29: Insulated heat storage. Adapted from Stamp and Majozi (2011)

The work reported by Seid and Majozi (2014) was aimed at proposing a heat integration framework, that can be used in conjunction with a scheduling formulation, and therefore, solving the combined formulation simultaneously, similar to the formulation of Stamp and Majozi (2011) . The work introduces the ability for a task to be integrated with another task at more than one time interval during its starting and finishing time. Stamp and Majozi (2011) had not accounted for temperature changes of the task between its starting and finishing times, i.e. at the intervals, which has been studied in the work by Seid and Majozi (2014). The formulation introduced the interval time point *pp* to account for these temperature changes within intervals. Considerations for indirect heat integration were also studied in the paper. The capacity of the storage and the initial temperature of the heat storage were determined by the model. The mathematical formulation resulted in a mixed integer nonlinear program which was linearized using Glover transformation (Glover, 1975) and reformulation linearization (Sherali & Alameddine, 1992).

A common heat exchanger network design for batch operations was proposed by Anastasovski (2014) using the time slice model. This was performed on a yeast and alcohol production plant. A common heat exchanger network was achieved with the basis of multipurpose use of heat exchanger as an operation philosophy. Anastasovski (2014) stated that there was a large area of heat exchangers that remains unused and aimed to maximise the use of the heat transfer area. A predetermined optimal schedule was used which was done using linear programming and simulated mathematical model. The heat exchanger that had the highest load was spilt into smaller heat exchangers with smaller heat transfer areas and capacities. The number of heat exchangers obtained was then minimized by taking all the duplicate heat exchangers as one. The heat exchangers were then redesigned and combined into a common heat exchanger network that was usable for all the time periods.

Castro et al. (2015) presented work that was aimed at optimising the schedule of single stage batch plants (meaning all subtasks occur in one unit) using direct heat integration. This was achieved through the use of a bi-objective model that will quantify the trade-off between the makespan and the utility consumption. The model development was separated into two parts namely; direct heat integration, and timing and sequencing of the production tasks. For the heat integration model, it was assumed that there would be a maximum of 2 stages for heating/cooling for each stream. The assumption was justified because in some instances a stage would be of a very short duration and therefore adding additional stages might result in more short duration matches. Due to the fact that there can be 2 stages of cooling/heating, an intermediate temperature and an intermediate time were defined. There were five different types of interactions which were identified by the Boolean variables (*ss, se, es, ee, no*). The rate of temperature change was also taken into account by the heat integration model.

The time and sequencing of production model by Castro et al. (2015) used the precedence time framework by Castro (2015) stated that the main difference between the precedence concept and the time slots was that the general precedence has explicit starting time variables for tasks whereas with time slots, the starting times are implicit. It was also stated that relating the starting times of a stream with its corresponding subtask is straightforward with general precedence models and general precedence models are easier to understand (Hajunkoski, et al., 2014). A zero wait operational philosophy was used. The disjunctions in the model were converted into MILP form. The bi-objective function was solved using an algorithm for generating Pareto set.

The proposed model presented by Castro et al. (2015) resulted in a clear trade-off between production time and utility consumption with energy savings ranging from 16% for the shortest production time to 40% savings for longer durations. It can also be concluded that higher energy savings can be achieved should the production schedule be even longer.

2.8.3. Heuristics and hybrid techniques

The seminal work done on heat integration in batch plants was by Vaselenak et al. (1986). The approach used temperature profiles and heuristics to determine the optimal heat integration of batch plants using hot and cold tanks. Three temperature profiles were studied which were co-current, counter-current and a combination of both co-current and counter-current nature. The equations which govern these temperature profiles were derived and outlined in the study. The equations derived for the counter-current temperature are similar to those used for continuous processes; therefore, the counter-current temperature profile was not studied due to the large extent of literature available.

The heat integration of batch processes can be of heuristic nature if the process does not possess any temperature limitations. The hot tanks are numbered in ascending order and cold tanks are numbered in descending order. The first hot tank is matched with the first cold tank but in order for heat to flow, the temperature of the hot tank must be greater than that of the cold tank plus the specified minimum difference in temperature called the minimum approach temperature (Vaselenak, et al., 1986). Any two tanks not violating this restriction can be paired and the temperature profile equations can be used to calculate the new temperatures of the tank after integration. Vaselenak et al. (1986) proved the validity of the heuristic approach using the cases of one hot tank and *n* cold tanks and one cold tank and *n* hot tanks.

De Boer et al. (2006) presented a case study that was performed on a process from the Dutch chemical company Dr. W. Kolb BV, for the evaluation of high temperature storage units. The process manufactures non-ionic tensides by alkoxylation of fatty alcohols and acids for use in detergents and cosmetics (De Boer, et al., 2006). The facility has two independent reactors in which an exothermic reaction takes place. The reactants of the exothermic reaction require preheating before the reaction occurs. After the exothermic reaction, different cooling stages then follow, which are dependent on the required temperature. There exists an opportunity for heat integration between the two reactors due to the fact that they operate in isolation of each other. The heat from the first reactor can be stored in the thermal storage vessel and then later used to preheat the reactants in the second reactor. Three storage tank options were considered. A tank filled with phase change materials with a melting point of 140^0C, a 20 ft tank filled with concrete with a bundle of 1800 tubes inside the concrete mass and a third tank that was a 45 ft container also filled with concrete and 1800 tubes were analysed. Direct heat integration was not taken into account and a single batch production was considered. The third storage tank option gave the highest savings on steam. This was because the storage capacity and the heat transfer of the storage tank matched the process requirements.

Holczinger et al. (2012) presented a study based on the S-graph approach proposed by Adonyi et.al. (2003) where it was assumed that heat exchangers were present for all hot-cold stream pairs and that each hot or cold stream was allowed to be matched with only one hot or cold stream. The aim of this work was to extend the work proposed by Adonyi et.al. (2003) by allowing the streams to have heat exchanges with multiple other streams and take into account the limitation on the number of available heat exchangers and their scheduling. The flow diagram of the formulation is as follows:

Proposed Approach

The proposed approach is a combination of linear programming tools and the S-graph framework. The problem was formulated as a MILP model and the branch and bound algorithm was then carried out through the S-graph approach. The bounds of the binary variables of the master MILP model was updated accordingly for each sub-problem. The relaxation of these MILP models was used to provide bounds at the internal nodes of the tree and the value of the solution at the leaves.

MILP master problem

The MILP master problem was based on the general precedence based formulation where binary variables were assigned to the allocation and sequencing of tasks, and the continuous variables represented the starting and finishing time of a task or material transfer. The constraints used for the MILP formulation were outlined in the paper.

S-graph based branching

The branch and bound algorithm was obtained through the extension of the S-graph based branching. The simple S-graph branching was represented with tasks and products as nodes.

For the extended representation, additional nodes can be added for transfer of materials, the intermediate material and the utility usage. In each step of the branch and bound procedure either a processing unit or a heat exchanger is scheduled. In both cases additional arcs are inserted to the graph.

Interaction between the MILP master problem and the S-graph framework

While the S-graph is being extended with the additional arcs throughout the branch and bound process, the MILP model is also being updated. This was done by setting the values of the binary variables that have been decided by the decisions made so far. The S-graph representation of the partial schedule provides additional information which can assist in solving the MILP model. If an MILP relaxation finds an integer optimal solution, no further branching is needed at that part of the tree.

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CHAPTER 3

MATHEMATICAL FORMULATION

3.1. Introduction

A mathematical formulation was proposed in which a variable schedule and energy usage is optimised simultaneously. The continuous time formation is used and the model can apply FIS operational philosophy. The proposed formulation is based on the superstructure depicted in Figure 3.1. This shows all the possible heat integration connections in the form of direct integration, indirect integration and the use of external utilities.

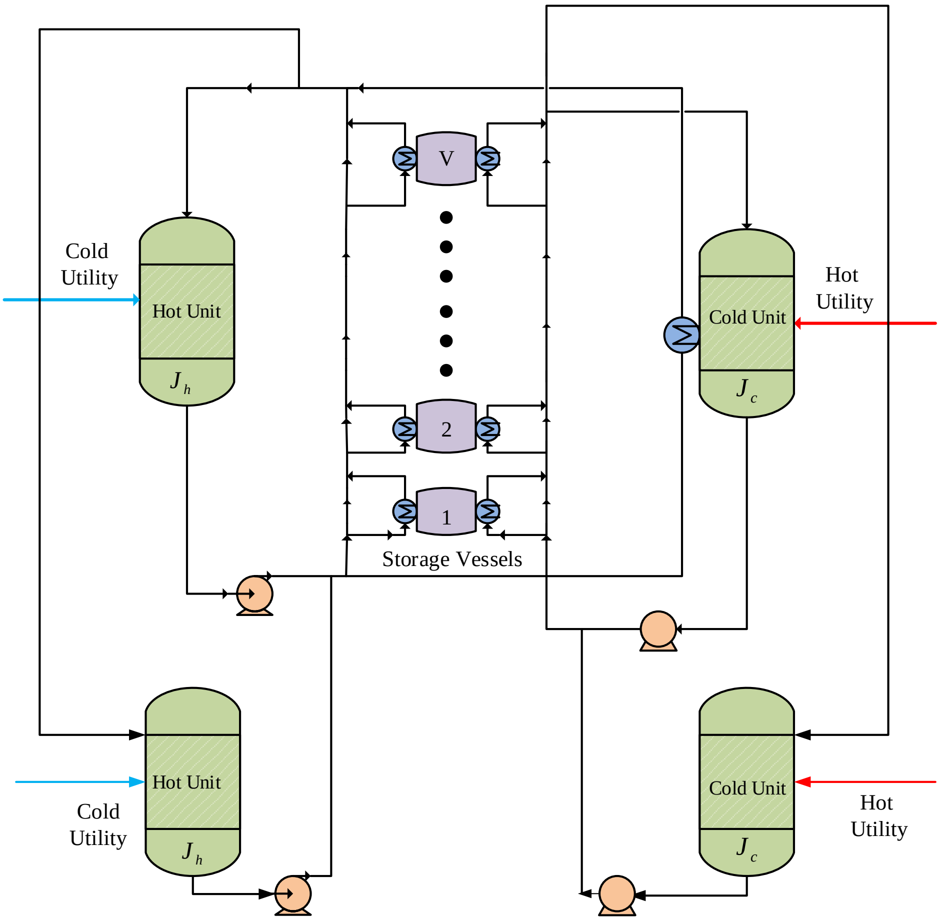

Figure 3.1: General superstructure for model development

3.2. Scheduling constraints

Scheduling constraints are critical in the mathematical formulation of batch processes. These constraints include capacity constraints of process units, duration constraints for the processing time, material balances for storage, sequence constraints, as well as allocation constraints of units. The scheduling formulation used is that of Seid and Majozi (2012), which employs a unit-specific model based on a continuous-time representation.

The scheduling formulation proposed by Seid and Majozi (2012) is based on finite intermidiate storage which means that intermidates arestored in storage vessels of a specific size. The formulation does not take into account the transfer times of materials from one unit to another and it also does not take into account the washing or cleaning operations between tasks. Seid and Majozi (2012) focused the proposed model in accurately addressing the storage constraints as well as proposing a formulation that could be solved in shorter CPU times. The proposed model allows for nonsimultaneous transfer of states. Nonsimultaneous transfer means that when a task requires more than one state, a state can be transfered to the unit in which it will be processed in and wait for the other state to be tranferred, then only can the task begin. The model is a base scheduling model which can then be used as foundation for heat integration or water minimisation.

3.3. Allocation constraints

Constraints (1) and (2) state that direct heat integration can take place between two units when the units are active. However, units can be active without direct heat integration taking place depending on the tasks that are conducted. These constraints work simultaneously to ensure that one unit which needs cooling will be integrated with one cold unit which needs heating at time point *p* in order for heat transfer to take place between the two units. It is important to note that heat transfer can take place between units that can perform multiple tasks. Although direct heat integration will take place between the units, integration will only take place when specific tasks within those units that can directly transfer heat to one another are active.

$$\sum_{s_{jc}^{in}} x\left(s_{jc}^{in}, s_{jh}^{in}, p\right) \leq y\left(s_{jh}^{in}, p\right) \qquad \forall s_{jh}^{in} \in S_{jh}^{in}, s_{jc}^{in} \in S_{jc}^{in}, p \in P \qquad (1)$$

$$\sum_{s_{jh}^{in}} x\left(s_{jc}^{in}, s_{jh}^{in}, p\right) \le y\left(s_{jc}^{in}, p\right) \qquad \forall s_{jh}^{in} \in S_{jh}^{in}, s_{jc}^{in} \in S_{jc}^{in}, p \in P \qquad (2)$$

Constraints (3) and (4) state that indirect heat integration can only take place between a task that requires heating or cooling and a heat storage vessel when that task is active. This ensures efficient heat transfer in that the heat transfer medium from a heat storage vessel will not heat or cool a unit when that unit is not active.

$$z\left(s_{jc}^{in}, v, p\right) \le y(s_{jc}^{in}, p) \qquad \forall, s_{jc}^{in} \in S_{jc}^{in}, p \in P \qquad (3)$$

$$z\left(s_{jh}^{in}, v, p\right) \le y(s_{jh}^{in}, p) \qquad \forall s_{jh}^{in} \in S_{jh}^{in}, p \in P \qquad (4)$$

Constraint (5) states that only one unit can be integrated with a heat storage vessel at time point *p*, and this condition applies to all heat storage vessels. One heat storage integration to one unit at a point in time will aid in simplifying process dynamics and promote efficient use of process resources. Constraint (5) is depicted in Figure 3.2.

$$\sum_{s_j^{in} \in S_{jc}^{in}} z\left(s_j^{in}, v, p\right) + \sum_{s_j^{in} \in S_{jh}^{in}} z\left(s_j^{in}, v, p\right) \le 1 \qquad \forall s_{jh}^{in} \in S_{jh}^{in}, s_{jc}^{in} \in S_{jc}^{in}, p \in P, \; v \in V \qquad (5)$$

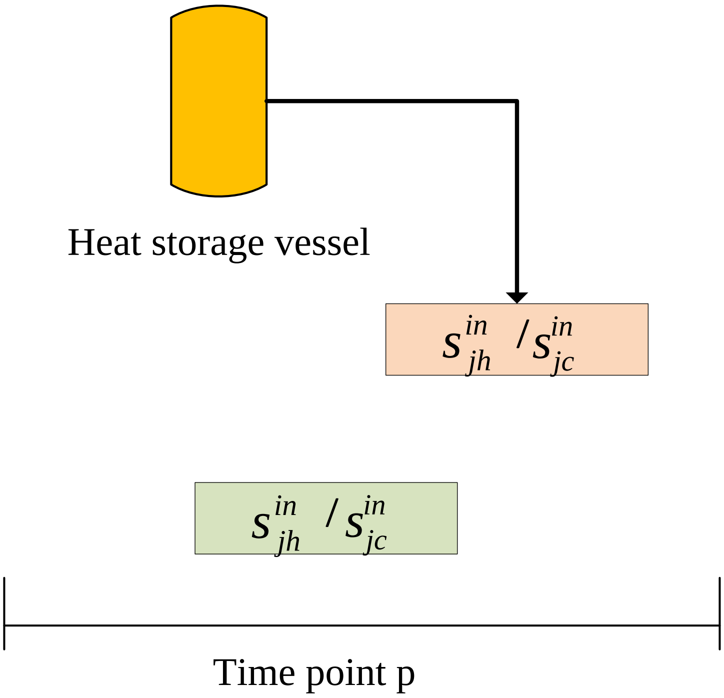

Figure 3.2: Indirect heat integration

Constraints (6) and (7) state that a unit can undergo either direct, $x\left(s_{jc}^{in}, s_{jh}^{in}, p\right)=1$, or indirect integration, , $z\left(s_{j}^{in}, v, p\right)=1$ at a point in time, and not both. This is so that the operation of the heat transfer between units is simplified and systematic.

$$\sum_{s_{jc}^{in}} x\left(s_{jc}^{in}, s_{jh}^{in}, p\right)+z\left(s_{jh}^{in}, v, p\right) \leq 1 \qquad \forall s_{jh}^{in} \in S_{jh}^{in}, s_{jc}^{in} \in S_{jc}^{in}, p \in P, v \in V \tag{6}$$

$$\sum_{s_{jh}^{in}} x\left(s_{jc}^{in}, s_{jh}^{in}, p\right)+z\left(s_{jc}^{in}, v, p\right) \leq 1 \qquad \forall s_{jh}^{in} \in S_{jh}^{in}, s_{jc}^{in} \in S_{jc}^{in}, p \in P, v \in V \tag{7}$$

3.4. Duties of tasks and heat storage vessels

Constraints (8) and (9) describe the amount of heat exchanged between a unit and a heat storage vessel for both cooling and heating by multiplying the mass of the heat transfer medium i.e. size of heat storage vessel with its heat capacity and the difference in temperature before and after integration has taken place Heat is transferred to or received from the heat storage vessel when the binary variable $z\left(s_{inj}, v, p\right)$ is equal to 1.

$$Q_c\left(s_{jc}^{in}, v, p\right)=W(v) c_p^w\left(T^i(v, p)-T^f(v, p)\right) z\left(s_{jc}^{in}, v, p\right) \qquad \forall s_{jc}^{in} \in S_{jc}^{in}, p \in P \tag{8}$$

$$Q_h\left(s_{jh}^{in}, v, p\right)=W(v) c_p^w\left(T^f(v, p)-T^i(v, p)\right) z\left(s_{jh}^{in}, v, p\right) \qquad \forall s_{jh}^{in} \in S_{jh}^{in}, p \in P \tag{9}$$

The duties of the heating and cooling tasks are obtained by using the difference between the supply temperatures and the target temperatures of the tasks. The duties are obtained in this way because the formulation is based on variable batch size that must be taken into account in determining the duties as the duties are a function of the batch size. The cooling duty is given by constraint (10) and the heating duty is given by constraint (11).

$$E_c\left(s_{jc}^{in}, p\right)=mu\left(s_{jc}^{in}, p\right) c_p\left(s_{jc}^{in}\right)\left(T^t\left(s_{jc}^{in}\right)-T^s\left(s_{jc}^{in}\right)\right) \qquad \forall s_{jh}^{in} \in S_{jh}^{in}, p \in P \tag{10}$$

$$E_h\left(s_{jh}^{in}, p\right)=mu\left(s_{jh}^{in}, p\right) c_p\left(s_{jh}^{in}\right)\left(T^s\left(s_{jh}^{in}\right)-T^t\left(s_{jh}^{in}\right)\right) \qquad \forall s_{jc}^{in} \in S_{jc}^{in}, p \in P \tag{11}$$

3.5. Design constraints

The upper and lower bounds of the initial temperatures of the heat storage vessels are defined by constraint (12). This constraint ensures that the heat storage vessels are always kept within the range of the operating temperatures of the heat storage vessels based on design characteristics such as material of construction.

$$T^L \le T^i(v,p) \le T^U \qquad \forall p \in P, v \in V \qquad (12)$$

Constraint (13) describes the size limits of the heat storage vessels. These limits ensure that the sizes of the heat storage vessels are practical. The decision variable e_{sto} in the constraint is used to denote the existence or non-existence of a heat storage vessel.

$$e_{sto}(v)W^L \le W(v) \le e_{sto}(v)W^U \qquad \forall v \in V \qquad (13)$$

3.6. Temperature constraints

The outlet temperature of any task at time point *p* should be equal to the specified target temperature of the task. This is described by constraints (14) and (15). The target temperature $T^t\left(s_j^{in}\right)$ is given as a parameter and the outlet temperature $T^{out}\left(s_j^{in}, p\right)$ is a variable. This aids the model in choosing the optimum points in time where a specific task should take place. This is described by constraints (14) and (15), shown in Figure 3.3.

$$T^{out}\left(s_{jc}^{in}, p\right) = T^t\left(s_{jc}^{in}\right) \qquad \forall s_{jc}^{in} \in S_{jc}^{in}, p \in P \qquad (14)$$

$$T^{out}\left(s_{jh}^{in}, p\right) = T^t\left(s_{jh}^{in}\right) \qquad \forall s_{jh}^{in} \in S_{jh}^{in}, p \in P \qquad (15)$$

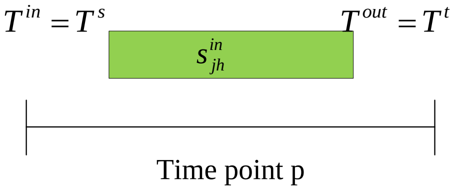

Figure 3.3: Temperature constraints for tasks

The inlet temperature of any task at time point *p* should be equal to the specified supply temperature of the task. This is described by constraints (16) and (17).

$$T^{in}\left(s_{jc}^{in}, p\right) = T^s\left(s_{jc}^{in}\right) \qquad \forall s_{jc}^{in} \in S_{jc}^{in}, p \in P \qquad (16)$$

$$T^{in}\left(s_{jh}^{in}, p\right) = T^s\left(s_{jh}^{in}\right) \qquad \forall s_{jh}^{in} \in S_{jh}^{in}, p \in P \qquad (17)$$

The initial temperature of a heat storage vessel at time point p must be equal to the final temperature of the heat storage vessel at time point p-1. This constraint assumes that the storage vessels are well insulated and no heat is lost to the environment.

$$T^{i}(v,p)=T^{f}(v,p-1) \qquad \forall p\in P, v\in V \tag{18}$$

Constraints (19) and (20) are related to constraint (18) and state that the temperature of the heat storage should not change when indirect heat integration does not take place. In a scenario where indirect heat integration takes place, then constraints (19) and (20) become redundant. These constraints are shown in Figure 3.4.

$$T^{f}(v,p)\leq T^{i}(v,p)+M\left(\sum_{s_{jc}^{in}} z\left(s_{jc}^{in},v,p\right)+\sum_{s_{jh}^{in}} z\left(s_{jh}^{in},v,p\right)\right) \qquad \forall s_{jh}^{in}\in S_{jh}^{in}, s_{jc}^{in}\in S_{jc}^{in}, p\in P, v\in V \tag{19}$$

$$T^{f}(v,p)\geq T^{i}(v,p)-M\left(\sum_{s_{jc}^{in}} z\left(s_{jc}^{in},v,p\right)+\sum_{s_{jh}^{in}} z\left(s_{jh}^{in},v,p\right)\right) \qquad \forall s_{jh}^{in}\in S_{jh}^{in}, s_{jc}^{in}\in S_{jc}^{in}, p\in P, v\in V \tag{20}$$

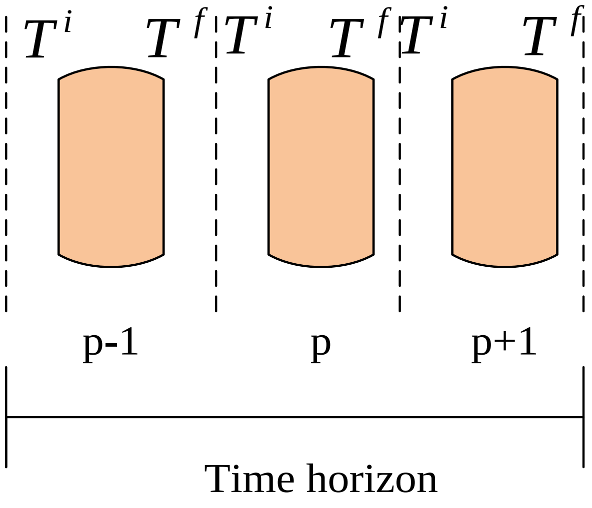

Figure 3.4: Temperature constraints for heat storage vessels

Constraints (21) and (22) ensure that for direct heat integration to take place, the minimum allowed temperature difference between the cold and hot units should be satisfied. The minimum allowable temperature difference ΔT^{L} is a parameter which is given depending on the process and it enables heat to be transferred between units efficiently because of the temperature difference that exists between units.

$$T^{in}\left(s_{jh}^{in}, p\right) - T^{out}\left(s_{jc}^{in}, p\right) \geq \Delta T^{L} - M\left(1 - x\left(s_{jc}^{in}, s_{jh}^{in}, p\right)\right) \qquad \forall s_{jh}^{in} \in S_{jh}^{in}, s_{jc}^{in} \in S_{jc}^{in}, p \in P \tag{21}$$

$$T^{out}\left(s_{jh}^{in}, p\right) - T^{in}\left(s_{jc}^{in}, p\right) \geq \Delta T^{L} - M\left(1 - x\left(s_{jc}^{in}, s_{jh}^{in}, p\right)\right) \qquad \forall s_{jh}^{in} \in S_{jh}^{in}, s_{jc}^{in} \in S_{jc}^{in}, p \in P \tag{22}$$

Constraints (23), (24), (25) and (26) ensure that for indirect heat integration to take place, the minimum temperature difference between a unit and a heat storage vessel should be satisfied for both cooling and heating.

$$T^{in}\left(s_{jh}^{in}, p\right) - T^{f}(v, p) \geq \Delta T^{L} - M\left(1 - z\left(s_{jh}^{in}, v, p\right)\right) \qquad \forall s_{jh}^{in} \in S_{jh}^{in}, s_{jc}^{in} \in S_{jc}^{in}, p \in P, v \in V \tag{23}$$

$$T^{out}\left(s_{jh}^{in}, p\right) - T^{i}(v, p) \geq \Delta T^{L} - M\left(1 - z\left(s_{jh}^{in}, v, p\right)\right) \qquad \forall s_{jh}^{in} \in S_{jh}^{in}, s_{jc}^{in} \in S_{jc}^{in}, p \in P, v \in V \tag{24}$$

$$T^{i}(v, p) - T^{out}\left(s_{jc}^{in}, p\right) \geq \Delta T^{L} - M\left(1 - z\left(s_{jc}^{in}, v, p\right)\right) \qquad \forall s_{jh}^{in} \in S_{jh}^{in}, s_{jc}^{in} \in S_{jc}^{in}, p \in P, v \in V \tag{25}$$

$$T^{f}(v, p) - T^{in}\left(s_{jc}^{in}, p\right) \geq \Delta T^{L} - M\left(1 - z\left(s_{jc}^{in}, v, p\right)\right) \qquad \forall s_{jh}^{in} \in S_{jh}^{in}, s_{jc}^{in} \in S_{jc}^{in}, p \in P, v \in V \tag{26}$$

3.7. Utility usage by tasks

The energy requirement of any task can be satisfied through three different mechanisms. These are indirect heat integration between a heat storage vessel and a task, direct heat integration between two tasks or external utilities depending on the energy requirement of the task. In a situation where energy requirements cannot be satisfied through direct and indirect heat integration, the use of external utilities is allowed to supplement the deficit. The aim of the formulation is to minimise the use of the external utilities. This is described by constraints (27) and (28), shown in Figure 3.5.

$$E_{h}\left(s_{jh}^{in}, p\right) y\left(s_{jh}^{in}, p\right) = \sum_{v} Q_{h}\left(s_{jh}^{in}, v, p\right) + c_{u}\left(s_{jh}^{in}, p\right) + \sum_{s_{jc}^{in}} Q_{e}\left(s_{jh}^{in}, s_{jc}^{in}, p\right) \qquad \forall s_{jh}^{in} \in S_{jh}^{in}, s_{jc}^{in} \in S_{jc}^{in}, p \in P, v \in V \tag{27}$$

$$E_{c}\left(s_{jc}^{in}, p\right) y\left(s_{jc}^{in}, p\right) = \sum_{v} Q_{c}\left(s_{jc}^{in}, v, p\right) + h_{u}\left(s_{jc}^{in}, p\right) + \sum_{s_{jh}^{in}} Q_{e}\left(s_{jh}^{in}, s_{jc}^{in}, p\right) \qquad \forall s_{jh}^{in} \in S_{jh}^{in}, s_{jc}^{in} \in S_{jc}^{in}, p \in P, v \in V \tag{28}$$

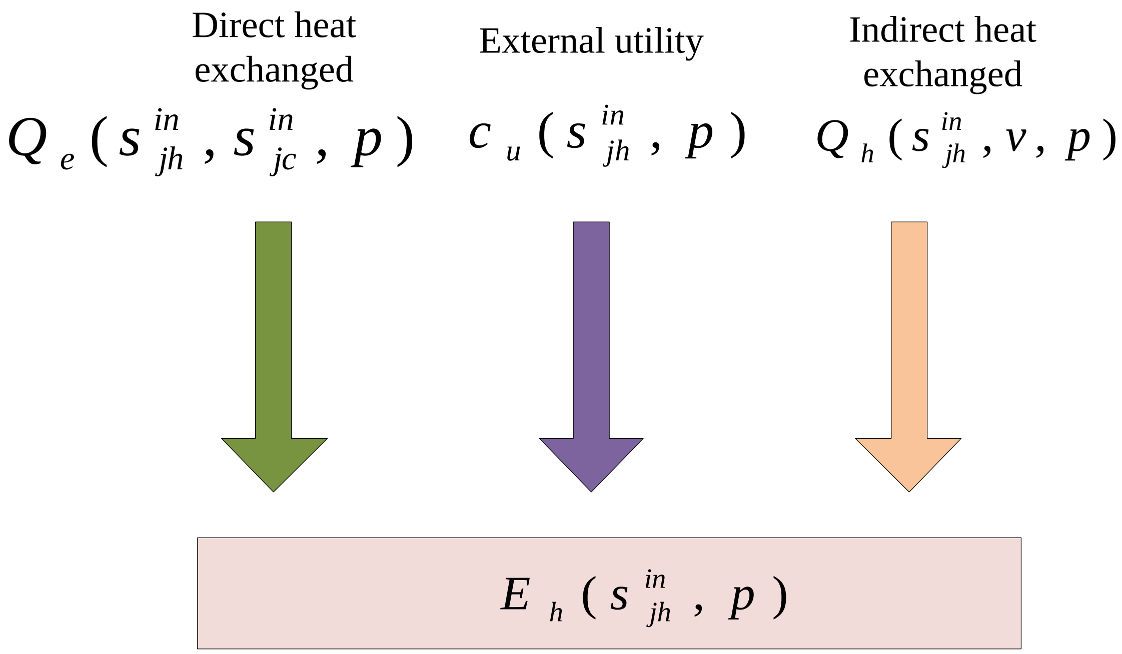

Figure 3.5: Utility usage constraint

3.8. Limits of heat exchanged during direct heat integration

Constraint (29) sets the bounds for the heat exchange between hot and cold tasks through direct heat integration. This ensures that amount of heat transferred between units is practical and is not insignificant or too large which can have a negative effect on the operating tasks.

$$Q_e^{\,L} x\left(s_{jc}^{in}, s_{jh}^{in}, p\right) \le Q_e\left(s_{jh}^{in}, s_{jc}^{in}, p\right) \le Q_e^{\,U} x\left(s_{jc}^{in}, s_{jh}^{in}, p\right) \qquad \forall s_{jh}^{in} \in S_{jh}^{in}, s_{jh}^{in} \in S_{jh}^{in}, p \in P \qquad (29)$$

3.9. Time constraints

When two units are directly integrated, the tasks of the units must start at the same time. Constraints (30) and (31) work together to ensure that integrated tasks start at the same time so that start of heat transfer between the two tasks can be at the same. The constraints become redundant when there is no integration i.e. $x\left(s_{jc}^{in}, s_{jh}^{in}, p\right) = 0$.

$$t_u\left(s_{jh}^{in}, p\right) \ge t_u\left(s_{jc}^{in}, p\right) - M\left(1 - x\left(s_{jc}^{in}, s_{jh}^{in}, p\right)\right) \qquad \forall s_{jh}^{in} \in S_{jh}^{in}, s_{jc}^{in} \in S_{jc}^{in}, p \in P \qquad (30)$$

$$t_u\left(s_{jh}^{in}, p\right) \le t_u\left(s_{jh}^{in}, p\right) + M\left(1 - x\left(s_{jc}^{in}, s_{jh}^{in}, p\right)\right) \qquad \forall s_{jh}^{in} \in S_{jh}^{in}, s_{jc}^{in} \in S_{jc}^{in}, p \in P \qquad (31)$$

Constraints (32), (33), (34) and (35) ensure that when integration takes place between a unit and a heat storage vessel, the starting times of the unit and the heat storage vessel must be equal. This ensures that heat transfer starts taking place as the tasks start. This applies for a unit requiring heating or cooling.

$$t_u\left(s_{jh}^{in},p\right)\geq t_o\left(s_{jh}^{in},v,p\right)-M\left(y\left(s_{jh}^{in},p\right)-z\left(s_{jh}^{in},v,p\right)\right) \qquad \forall s_{jh}^{in}\in S_{jh}^{in}, s_{jc}^{in}\in S_{jc}^{in}, p\in P, v\in V \tag{32}$$

$$t_u\left(s_{jh}^{in},p\right)\leq t_o\left(s_{jh}^{in},v,p\right)+M\left(y\left(s_{jh}^{in},p\right)-z\left(s_{jh}^{in},v,p\right)\right) \qquad \forall s_{jh}^{in}\in S_{jh}^{in}, s_{jc}^{in}\in S_{jc}^{in}, p\in P, v\in V \tag{33}$$

$$t_u\left(s_{jc}^{in},p\right)\geq t_o\left(s_{jc}^{in},v,p\right)-M\left(y\left(s_{jc}^{in},p\right)-z\left(s_{jc}^{in},v,p\right)\right) \qquad \forall s_{jh}^{in}\in S_{jh}^{in}, s_{jc}^{in}\in S_{jc}^{in}, p\in P, v\in V \tag{34}$$

$$t_u\left(s_{jc}^{in},p\right)\leq t_o\left(s_{jc}^{in},v,p\right)+M\left(y\left(s_{jc}^{in},p\right)-z\left(s_{jc}^{in},v,p\right)\right) \qquad \forall s_{jh}^{in}\in S_{jh}^{in}, s_{jc}^{in}\in S_{jc}^{in}, p\in P, v\in V \tag{35}$$

Constraints (36), (37), (38) and (39) are similar to constraints (32)-(35) but apply to the finishing time of a task and the corresponding heat storage unit. They ensure that the finishing time of a task and the finishing time of the heat storage vessel are equal when indirect integration takes place between a task and a heat storage vessel.

$$t_p\left(s_{jh}^{in},p\right)\geq t_f\left(s_{jh}^{in},v,p\right)-M\left(y\left(s_{jh}^{in},p\right)-z\left(s_{jh}^{in},v,p\right)\right) \qquad \forall s_{jh}^{in}\in S_{jh}^{in}, s_{jc}^{in}\in S_{jc}^{in}, p\in P, v\in V \tag{36}$$

$$t_p\left(s_{jh}^{in},p\right)\leq t_f\left(s_{jh}^{in},v,p\right)+M\left(y\left(s_{jh}^{in},p\right)-z\left(s_{jc}^{in},v,p\right)\right) \qquad \forall s_{jh}^{in}\in S_{jh}^{in}, s_{jc}^{in}\in S_{jc}^{in}, p\in P, v\in V \tag{37}$$

$$t_p\left(s_{jc}^{in},p\right)\geq t_f\left(s_{jc}^{in},v,p\right)-M\left(y\left(s_{jc}^{in},p\right)-z\left(s_{jc}^{in},v,p\right)\right) \qquad \forall s_{jh}^{in}\in S_{jh}^{in}, s_{jc}^{in}\in S_{jc}^{in}, p\in P, v\in V \tag{38}$$

$$t_p\left(s_{jc}^{in},p\right)\leq t_f\left(s_{jc}^{in},v,p\right)+M\left(y\left(s_{jc}^{in},p\right)-z\left(s_{jc}^{in},v,p\right)\right) \qquad \forall s_{jh}^{in}\in S_{jh}^{in}, s_{jc}^{in}\in S_{jc}^{in}, p\in P, v\in V \tag{39}$$

These constraints ensure that a heat storage vessel is active for the duration of a task that it is integrated with at time point *p-1* before it can be active again for integration of the same task in a different unit at time point *p*. Constraint (40) applies to tasks that need heating and constraint (41) describes tasks that need cooling.

$$t_o(s_{jc}^{in},v,p)\geq t_o(s_{jc'}^{in},v,p-1)+ \alpha(s_{jc'}^{in})y(s_{jc'}^{in},p-1)+\beta(s_{jc'}^{in})mu(s_{jc'}^{in},p-1) \qquad \forall s_{jh}^{in}\in S_{jh}^{in}, s_{jc}^{in}\in S_{jc}^{in}, p\in P, v\in V \tag{40}$$

$$t_o(s_{jh}^{in}, v, p) \geq t_o(s_{jh'}^{in}, v, p-1) + \alpha(s_{jh'}^{in}) y(s_{jh'}^{in}, p-1) + \beta(s_{jh'}^{in}) mu(s_{jh'}^{in}, p-1) \quad \forall s_{jh}^{in} \in S_{jh}^{in}, s_{jc}^{in} \in S_{jc}^{in}, p \in P, v \in V \tag{41}$$

Constraints (42) and (43) are the same as constraints (40) and (41) but apply in a situation where a heat storage vessel is integrated with different units, depicted in Figure 3.6.

$$t_o(s_{jh}^{in}, v, p) \geq t_o(s_{jc}^{in}, v, p-1) + \alpha(s_{jc}^{in}) y(s_{jc}^{in}, p-1) + \beta(s_{jc}^{in}) mu(s_{jc}^{in}, p-1) \quad \forall s_{jh}^{in} \in S_{jh}^{in}, s_{jc}^{in} \in S_{jc}^{in}, p \in P, v \in V \tag{42}$$

$$t_o(s_{jc}^{in}, v, p) \geq t_o(s_{jh}^{in}, v, p-1) + \alpha(s_{jh}^{in}) y(s_{jh}^{in}, p-1) + \beta(s_{jh}^{in}) mu(s_{jh}^{in}, p-1) \quad \forall s_{jh}^{in} \in S_{jh}^{in}, s_{jc}^{in} \in S_{jc}^{in}, p \in P, v \in V \tag{43}$$

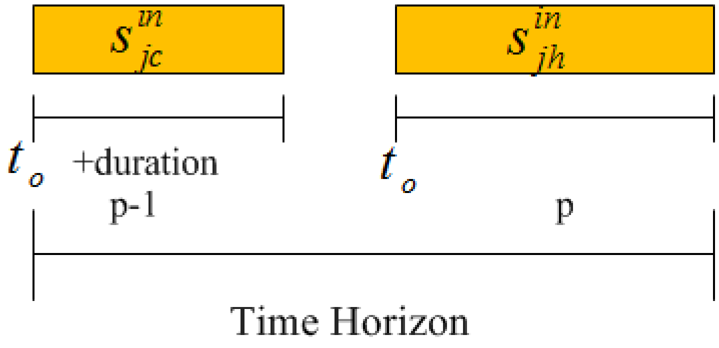

Figure 3.6: Time constraints

3.10. Objective function

The objective of the model is to maximize profit in the batch process which constitutes of the revenue from the products, cost of external cold utility and hot utility defined as cu_c and hu_c, respectively, and the capital cost of the heat storage vessels which was omitted from the indirect heat integration formulation of Stamp and Majozi (2011). The cost function of the heat storage vessels is nonlinear and was obtained from the work of Li and Chang (2006). The plant is assumed to be operational for 7920 hours per year while the exponent of the cost function is assumed to be 0.6. The objective function is given by constraint (44) and the annualizing factor is given by constraint (45) obtained from Foo (2010) where the annual fractional interest rate is assumed to be 15% and lifespan of the heat storage vessels is 3 years.

$$\max\left(\begin{array}{l}(\sum_{s_p} qs(s_p,p)SP(s_p) - \sum_{p}\sum_{s_{jh}^{in}} c_u(s_{jh}^{in},p)cu_c \\ -\sum_{p}\sum_{s_{jc}^{in}} h_u(s_{jc}^{in},p)hu_c)\dfrac{hr/yr}{H} \\ -\sum_{v}((\alpha_{sto}+\beta_{sto}W(v)^{\theta})e_{sto}(v))A^F\end{array}\right) \qquad \forall s_p \in S_P, s_{jh}^{in} \in S_{jh}^{in}, s_{jc}^{in} \in S_{jc}^{in}, p \in P, v \in V \tag{44}$$

$$A^F = \frac{a(1+a)^n}{(1+a)^n - 1} \tag{45}$$

3.11. Nomenclature

The following sets, variables and parameters are used in the formulation.

Sets

J	$\{j \mid j$ processing unit$\}$
J_c	$\{j_c \mid j_c$ cold processing unit$\}$
J_h	$\{j_h \mid j_h$ hot processing unit$\}$
P	$\{p \mid p$ time point$\}$
S_{jh}^{in}	$\{s_{jh}^{in} \mid s_{jh}^{in}$ task which needs cooling$\}$
S_{jc}^{in}	$\{s_{jc}^{in} \mid s_{jc}^{in}$ task which needs heating$\}$
S_j^{in}	$\{s_j^{in} \mid s_j^{in}$ any task$\}$
S_p	$\{s_p \mid s_p$ any product$\}$
V	$\{v \mid v$ is a heat storage vessel$\}$

Variables

$E_c(s_{jc}^{in},p)$	duty of task which needs heating
$E_h(s_{jh}^{in},p)$	duty of task which needs cooling
$c_u(s_{jh}^{in},p)$	cooling water required by a hot task
$h_u(s_{jc}^{in},p)$	steam required by a cold task
$mu(s_{jc}^{in},p)$	amount of material processed by cold task
$mu(s_{jh}^{in},p)$	amount of material processed by hot task
$T^i(v,p)$	initial temperature of a storage vessel
$T^f(v,p)$	final temperature of a storage vessel
$T^{out}(s_{jc}^{in},p)$	outlet temperature of a cold task
$T^{out}(s_{jh}^{in},p)$	outlet temperature of a hot task
$T^{in}(s_{jc}^{in},p)$	inlet temperature of a cold task
$T^{in}(s_{jh}^{in},p)$	inlet temperature of a hot task
$t_u(s_{jc}^{in},p)$	time at which a cold task starts being active

$t_u(s_{jh}^{in}, p)$	time at which a hot task starts being active
$t_p\left(s_{jc}^{in}, p\right)$	time at which a cold task stops being active
$t_p\left(s_{jh}^{in}, p\right)$	time at which a hot task stops being active
$t_o(s_{jc}^{in}, v, p)$	time at which a heat storage starts being active when integrated with a cold task
$t_o(s_{jh}^{in}, v, p)$	time at which a heat storage starts being active when integrated with a hot task
$t_f(s_{jc}^{in}, v, p)$	time at which a heat storage stops being active when integrated with a cold task
$t_f(s_{jh}^{in}, v, p)$	time at which a heat storage stops being active when integrated with a hot task
$qs(s_p, p)$	amount of product at the end of the time horizon
$Q_c(s_{jc}^{in}, v, p)$	heat transferred from storage to cold task
$Q_h(s_{jh}^{in}, v, p)$	heat transferred from hot task to storage
$Q_e(s_{jh}^{in}, s_{jc}^{in}, p)$	amount of heat directly transferred between a hot and cold task
$W(v)$	capacity of heat storage
$e_{sto}(v)$	binary variable indicating the existence of a heat storage vessel
$x(s_{jc}^{in}, s_{jh}^{in}, p)$	binary variable indicating direct integration between a hot and cold task
$y(s_{jc}^{in}, p)$	binary variable indicating an active cold task
$y(s_{jh}^{in}, p)$	binary variable indicating an active hot task
$z(s_{jc}^{in}, v, p))$	binary variable indicating an active heat storage vessel integrated with a cold task
$z(s_{jh}^{in}, v, p))$	binary variable indicating an active heat storage vessel integrated with a hot task

Parameters

α_{sto}	fixed cost of heat storage vessel
β_{sto}	variable cost of heat storage vessel
$\alpha(s_j^{in})$	coefficient of constant term for processing time of a task
$\beta(s_j^{in})$	coefficient of variable term for processing time of a task
A^F	annualizing factor
a	annual fractional interest rate
θ	cost function exponent
$c_p(s_{jc}^{in})$	specific heat capacity of a cold task
$c_p(s_{jh}^{in})$	specific heat capacity of a hot task
C_p^w	specific heat capacity of heat transfer medium
cu_c	cost of cold utility
hu_c	cost of hot utility
hr/yr	amount of hours the plant operates per year

H	time horizon of interest
M	Any large number
n	lifespan of heat storage vessels in years
$SP(s_p)$	selling price of products
$T^s(s^{in}_{jh})$	inlet temperature of a hot task
$T^s(s^{in}_{jc})$	Inlet temperature of a cold task
$T^t(s^{in}_{jh})$	outlet temperature of hot task
$T^t(s^{in}_{jc})$	outlet temperature of a cold task
$\boldsymbol{T}^L$	lower bound for initial temperature of a heat storage vessel
$\boldsymbol{T}^U$	upper bound for initial temperature of a heat storage vessel
ΔT^L	minimum allowable temperature difference
W^L	lower bound for size of a heat storage vessel
W^U	upper bound for size of a heat storage vessel
Q_e^L	lower bound for amount of heat transferred between two tasks
Q_e^U	upper bound for amount of heat transferred between two tasks

3.12. References

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CHAPTER 4

ILLUSTRATIVE EXAMPLES

4.1. Introduction

The mathematical formulation was applied to two illustrative examples adapted from Majozi (2010) and Kondili et al. (1993). The examples involve multipurpose batch plants which have tasks that require either heating or cooling. The models were solved in GAMS 24.3.2 using the general purpose global optimisation solver BARON in Intel® Core™ i7-3770 CPU @ 3.40 GHz, RAM 8.00 GB.

4.2. First illustrative example (adapted from Majozi (2010))

A batch plant which consists of two reactors, two filters and a distillation column was considered for the first example. The recipe, that is the procedure that must be followed in order to convert the raw materials to the final products, is represented as a state sequence network (SSN) in Figure 4.1. SSN is a representation of the recipe as a diagram. The materials/states used in the process such as raw materials, intermediates, waste products and products are used in the sequence and the processes/tasks which take place i.e. reaction, filtration are denoted as nodes. The mass fraction of the states used to perform a certain task is also denoted on the SSN in order in quantify the amount of state used for each task. The first illustrative example consists of three main tasks which is reaction, filtration and distillation/separation. The reaction task can take place in either reactor 1 or 2, using state 1 and 2 as raw materials to produce state 3and needs to be cooled from 100°C to 70°C. The filtration task can be carried out in filters 1 and 2 where state 3 is filtered to obtain state 4 and state 5 which is a waste product. The separation task distils state 4 into state 6 and 7 is carried out in the distillation column and should be heated from 65°C to 80°C. Figure 4.2(a) shows the process flow diagram of the illustrative example.

The reaction task is 2 hours long and a maximum batch size of 60 kg can be produced in each reactor. The filtration is 1 hour long and can handle a maximum batch size of 80 kg as its feed. The distillation task is 2 hours long and takes a maximum batch size of 140 kg as the feed to the distillation column. The batch plant has a tank farm where each state used or produced from the process can be stored. The maximum storage capability of the intermediate states is shown in Figure 4.2(b). The initial inventory of the raw materials, state 1 and 2 is given as 1000 kg each at the start of production

The detailed scheduling data and the detailed heating/cooling requirement data is given in Tables 4.3, 4.4 and 4.5, and the detailed heat storage vessel cost function parameters are given in Table 4.6 in Appendix A. The superstructure of the example is given in Figure 4.3. The superstructure had a maximum of four heat storage vessels which could be used for indirect heat integration together with opportunities for direct heat integration and the use of external utilities.

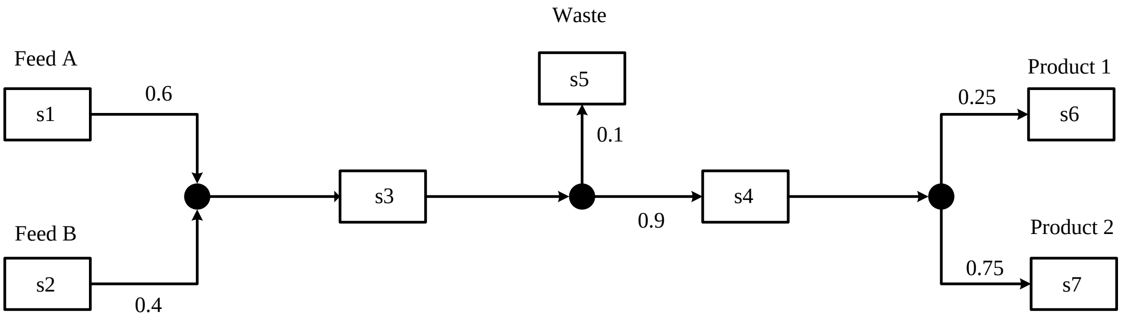
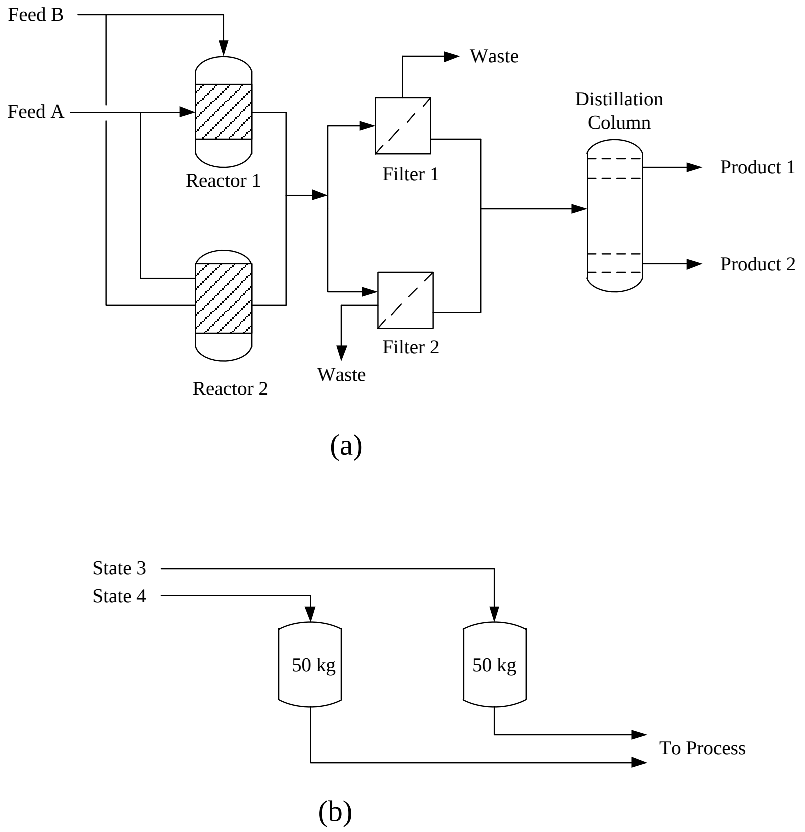


Figure 4.1: SSN for first illustrative example



(a)

(b)

Figure 4.2: (a) Process Flow Diagram, (b) Tank Farm for first illustrative example

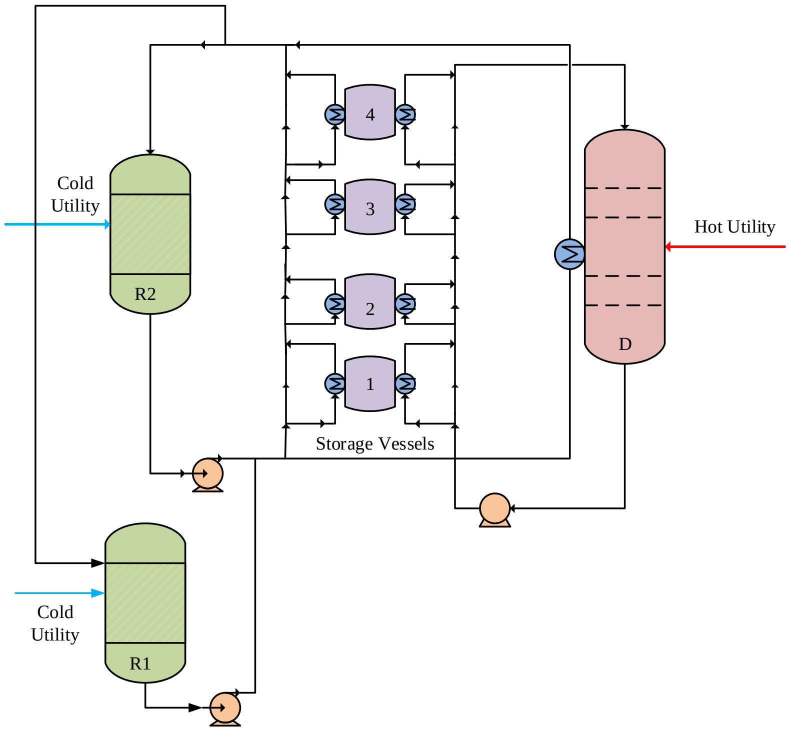


Figure 4.3: Superstructure for first illustrative example

Three different scenarios of the illustrative example were considered. The first scenario (scenario 1) is a base case where there is no heat integration. The second scenario (scenario 2) is a single heat storage vessel model together with direct heat integration opportunities and the third scenario (scenario 3) involves multiple heat storage vessels. The selling price for products 1 and 2 is c.u 120 and the cost of the cold and hot utilities is c.u 0.02 and c.u 1, respectively. The model was applied to the example and the results were analysed and compared.

4.2.1 Results and discussion

The results obtained from the application of the model are given in Table 4.1. The objective value obtained for scenario 1 was c.u 31.4x10^6. This is mainly due to the fact that only three main tasks take place in the process. Two of those tasks require heating/cooling and as such a huge amount of external utilities is used for the first scenario. Scenario 2 resulted in an objective value of c.u 33.5x10^6. The hot utility was eliminated and the cold utility requirement was 50.40 MJ. Scenario 3 resulted in an objective value of c.u 34.1x10^6 and no external utilities requirements.

The proposed mathematical formulation resulted in an optimal number of three heat storage vessels which are depicted in the resultant flowsheet in Figure 4.4. The flowsheet shows that the model achieves its optimal objective value when only indirect heat integration occurs. It should be noted that 100% decrease of external utilities does not take into account the cold and hot utilities that are used in the heat storage vessels to achieve the initial temperatures although the cost of the heat transfer medium is taken into account with the cost of storage. The objective value of the scheduling model, where no utilities are considered, was found to be c.u 34.2x10^6 and scenario 3 (multiple heat storage vessels model) resulted in an objective of c.u 34.1x10^6. It can be seen that the multiple heat storage vessels model achieved an objective value closest to the scheduling model objective value, as compared to scenario 1 and 2. This shows that the proposed mathematical formulation not only minimises the use of external utilities, but also allows for flexibility with regards to time. This means that more batches can be produced within the time horizon as though utilities were not considered like in the scheduling model. The objective value of the proposed model is however not equal to the scheduling objective value because the capital costs of the heat storage vessels were accounted for in the objective function of multiple heat storage vessels model, whereas the scheduling model takes into account the amount of product with its selling price only.

It is evident that the heat integration configuration of the heat storage vessels resulted in one heat storage being used to heat the distillation task, while the other two heat storage vessels were used to cool down the reaction task in both reactors as illustrated in the Gantt chart in Figure 4.5. For this specific example, the configuration of using all heat storage vessels as both sinks and sources was not the best solution. This can be attributed to the fact that there were only two tasks which required external utilities, therefore segregating the usage of heat storage vessels to suit the needs of the tasks resulted in a simpler heat exchange configuration. The initial temperatures of the heat storage vessels also affect the type of configuration output.

The heat storage vessels had initial temperatures of 20°C, 20°C and 160°C and sizes of 112.5 kg, 150 kg and 116.2 kg. The temperature profiles of the heat storage vessels are depicted in Figure 4.6 which show the changes in temperature of each of the heat storage vessels throughout the time horizon. The heat loss of the heat storage vessels was not considered due to the short length of the time horizon. Due to the nonlinear nature of the model and the computational intensity required in solving it, the CPU time was set at a limit of 6000 s for the single heat storage vessel and the multiple heat storage vessel scenarios. Given that the problem being solved is a design problem a longer CPU time can be tolerated.

Piping costs were not taken into account in the mathematical formulation. Figure 4.7 shows the configuration of a unit with the heat exchanger used to facilitate heat transfer. The unit will have standard piping whether the heat transfer medium is from external utilities, direct or indirect heat integration. The additional piping costs will come from each heat storage vessel added to the heat transfer configuration through indirect heat integration as shown in Figure 4.7. The total cost of piping can then be minimised by optimally arranging the configuration of the heat storage vessels and the units.

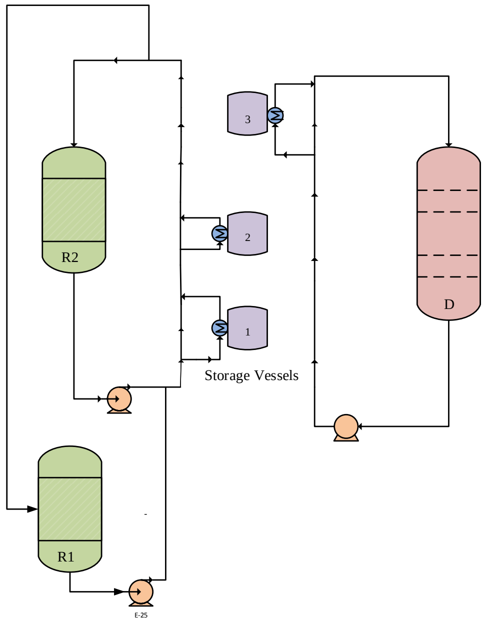


Figure 4.4: Resultant flowsheet for first illustrative example

Table 4.1: Results for first illustrative example

	No integration	One heat storage vessel	Multiple heat storage vessels
Objective (c.u x 10^6)	31.4	33.5	34.1
Cold utility (MJ)	50.4	50.40	0
Hot utility (MJ)	41.47	0	0
Discrete variables	70	101	253
Continuous variables	265	429	1117
Time points	6	6	6
CPU time (s)	1	6000	6000

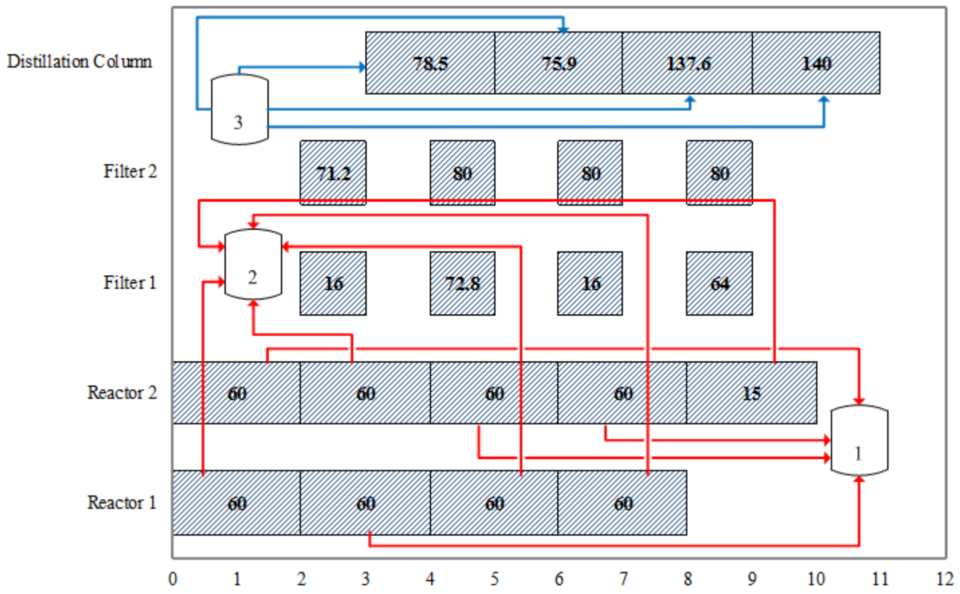


Figure 4.5: Gantt chart using proposed model for first illustrative example showing the schedule of the batch process

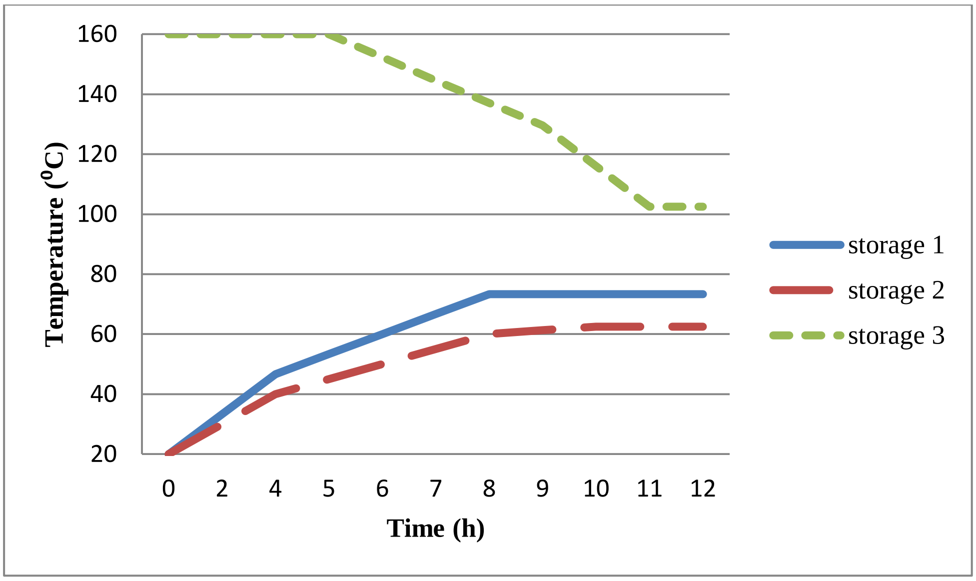


Figure 4.6: Temperature profile for heat storage vessels for first illustrative example

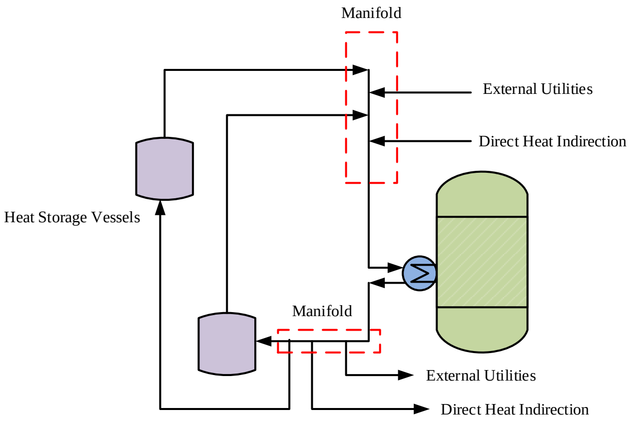


Figure 4.7: Piping design of a heat storage vessel showing the use of utilities

4.3. Second illustrative example (adapted from Kondili et al. (1993))

A multipurpose batch plant which consists of a heater, two reactors, in which three reactions can occur and a separation unit was also considered. The recipe is represented as a State Sequence Network (SSN) in Figure 4.8 which shows the procedural steps of the process. The SSN is represented in the same way as in the first illustrative example. The second illustrative example consists of heating, three reaction steps and separation. The heat task heats state 1 to produce state 5. Reaction 1 task reacts state 2 and 3 to produce state 6 and must be cooled from 100°C to 70°C. Reaction 2 reacts state 5 and 6 to produce state 7, which is product 1 and state 8 and must be heated from 70°C to 100°C. Reaction 3 reacts state 4 and 8 to produce state 9 and must be cooled from 130°C to 100°C. The separation task separates state 9 into state 10, which is product 2, and state 8 which is recycled back to be used for reaction 3. Figure 4.9(a) shows the process flow diagram of the illustrative example.

The duration of all tasks varies depending on the quantity of the batch being processed or produced. The constants used to determine the duration of the batches can be found in Appendix A. The maximum batch size that can be heated for the heating task is 100 kg. The maximum batch size to be produced in reactors 1 and 2 is 50 kg and 80 kg, respectively. The separation can handle a maximum of 200 kg of feed to be separated. The tank farm which shows the maximum storage capability of the intermediate states is shown in Figure 4.9(b). The initial inventory of the raw materials, states 1, 2, 3 and 4 is given as 1000 kg each at the start of production.

The detailed scheduling data and the detailed heating/cooling requirement data is given in Tables 4.7, 4.8 and 4.9, and the detailed heat storage vessel cost function parameters are given in Table 4.10 in Appendix A. The three scenarios considered for the first example were once again considered for the second example namely; base case scenario (scenario 1), one heat storage vessel (scenario 2) as well as multiple heat storage vessels (scenario 3). The superstructure for the example is given in Figure 4.10. The superstructure had a maximum of five heat storage vessels which could be used for indirect heat integration together with opportunities for direct heat integration and the use of external utilities. The selling price for products 1 and 2 is c.u 20 and the cost of the cold and hot utilities is c.u 0.02 and c.u 1, respectively.

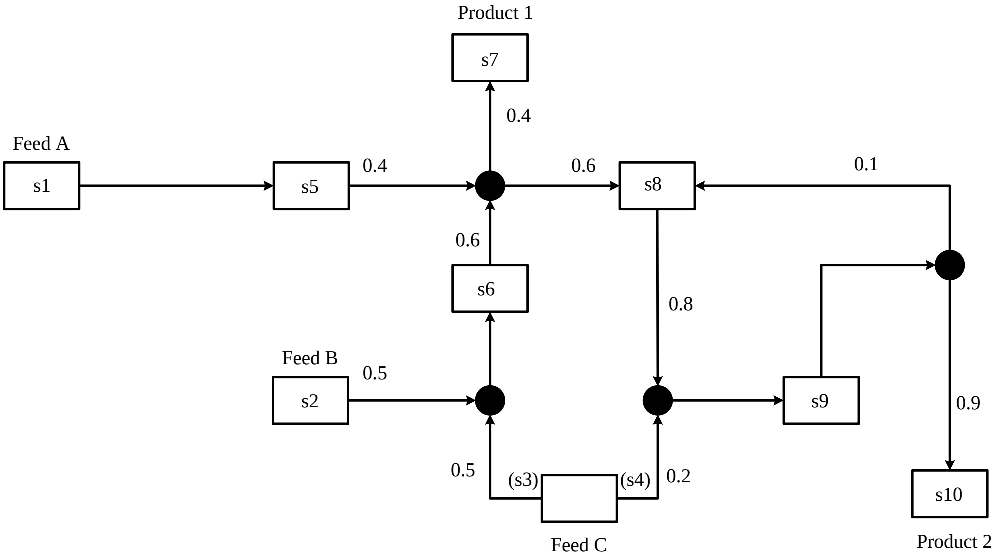
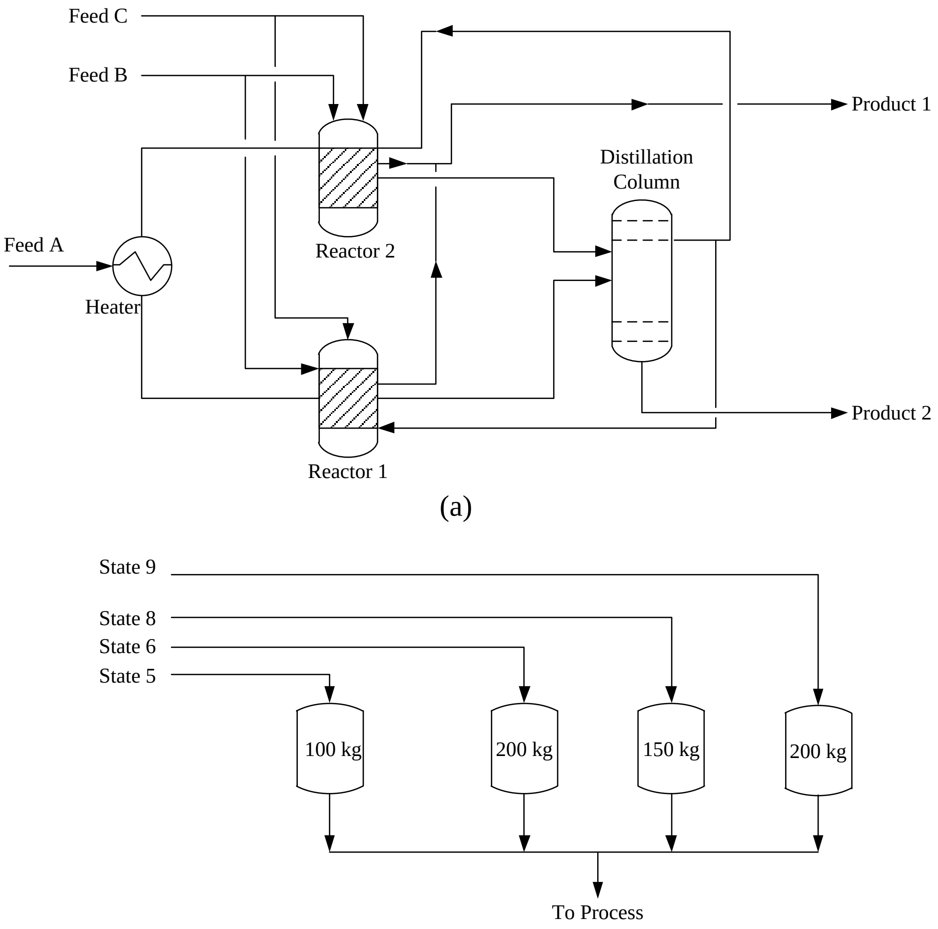


Figure 4.8: SSN for second illustrative example



(a)

(b)

Figure 4.9: (a) Process Flow Diagram, (b) Tank Farm for second illustrative example

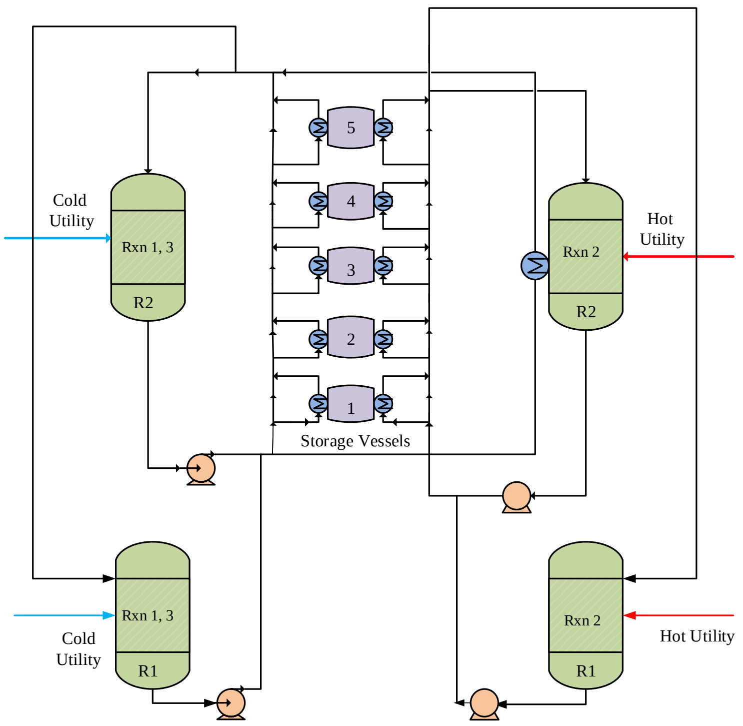


Figure 4.10: Superstructure for second illustrative example

4.3.1 Results and discussion

The resultant flowsheet and the Gantt chart with the heat integration configuration are presented in Figures 4.11 and 4.12, respectively. Scenario 1 resulted in an objective value of c.u 465.2x10^3, hot utility requirement of 16.6 MJ and cold utility requirement of 21 MJ for a 10 hour time horizon. Scenario 2 resulted in an increased objective value of c.u 2.5x10^6 and a cold utility of 15.6 MJ. A further increase in the objective value (c.u 2.9x10^6) was achieved for scenario 3. No external utilities were used when the proposed model was applied to the illustrative example. This demonstrates that the application of multiple heat storage results not only in the decrease of operational costs, in this instance external utilities, but can result in flexibility of time in the plant which will ultimately affect the revenue of the plant. There is trade-off between cost of the heat storage vessels and minimisation of energy using indirect heat integration. The results of the proposed model show that high savings in external utilities can still be achieved even with the consideration of the capital cost of the storage vessels. The results for the proposed formulation are given in Table 4.2.

The proposed model achieved an optimal number of four heat storage vessels together with the optimal sizes of 25.7 kg, 25.6 kg, 36.6 kg and 22.9 kg respectively. The optimal initial temperatures of the vessels were 20°C, 20°C, 160°C and 160°C respectively. The temperature profiles of the heat storage vessels for the 10 hour time horizon are depicted in Figure 4.13.

It is worth mentioning that although direct integration was considered in the mathematical formulation, the model did not yield any direct integration connections but integration took place through indirect integration only. This is due to the fact that direct integration places stringent time constraints on the tasks. With the use of multiple heat storage vessels, greater flexibility in terms of time is achieved in the plant, which surpasses that of one heat storage vessel and this is evident from the results obtained after the application of the mathematical model to the illustrative example. The CPU time was once again set at a limit of 6000 s for both scenario 2 and 3.

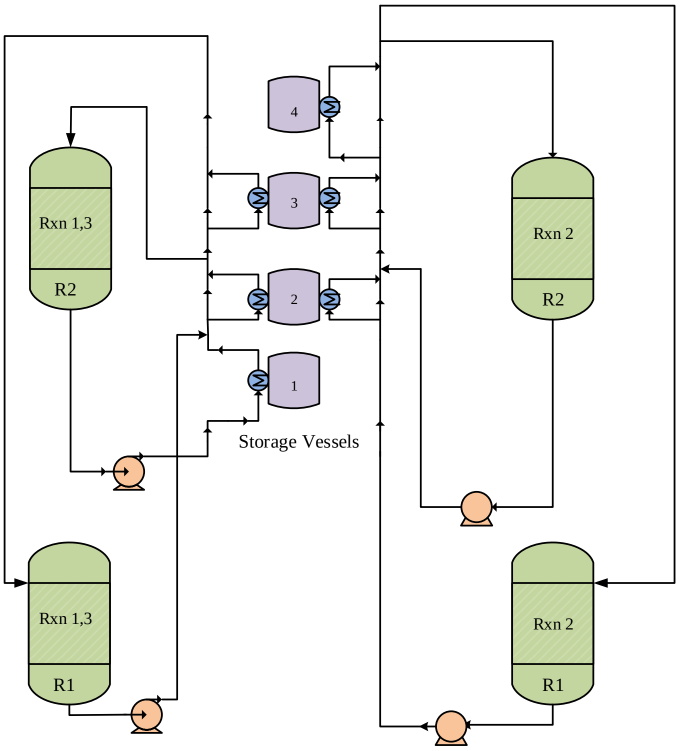


Figure 4.11: Resultant flowsheet for second illustrative example

Table 4.2: Results for second illustrative example

	No integration	One heat storage vessel	Multiple heat storage vessels
Objective (c.u)	465.2×10^3	$2{,}5 \times 10^6$	$2{,}9 \times 10^6$
Cold utility (MJ)	21.0	15.6	0
Hot utility (MJ)	16.6	0	0
Discrete variables	72	143	236
Continuous variables	337	639	1035
Time points	5	5	5
CPU time (s)	3	6000	6000

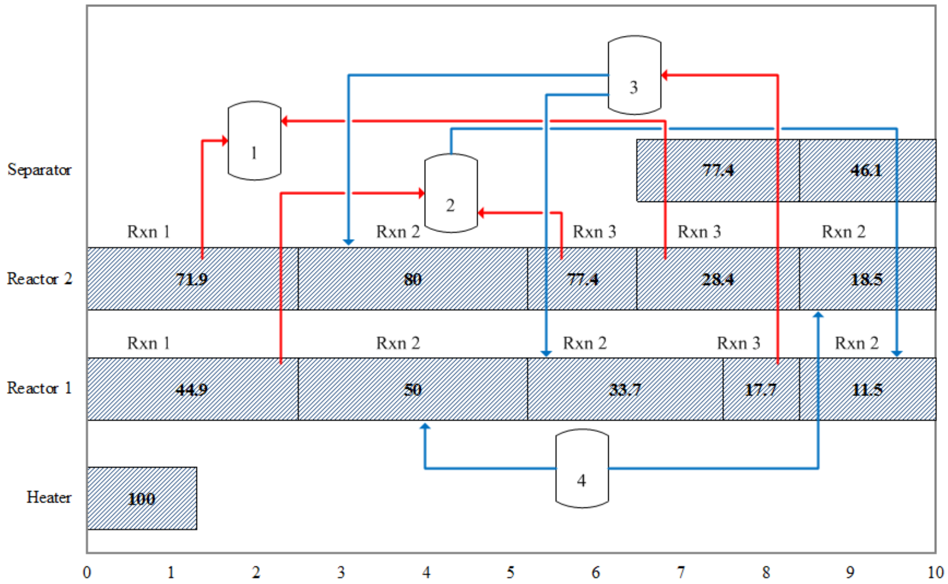


Figure 4.12: Gantt chart using proposed model for second illustrative example

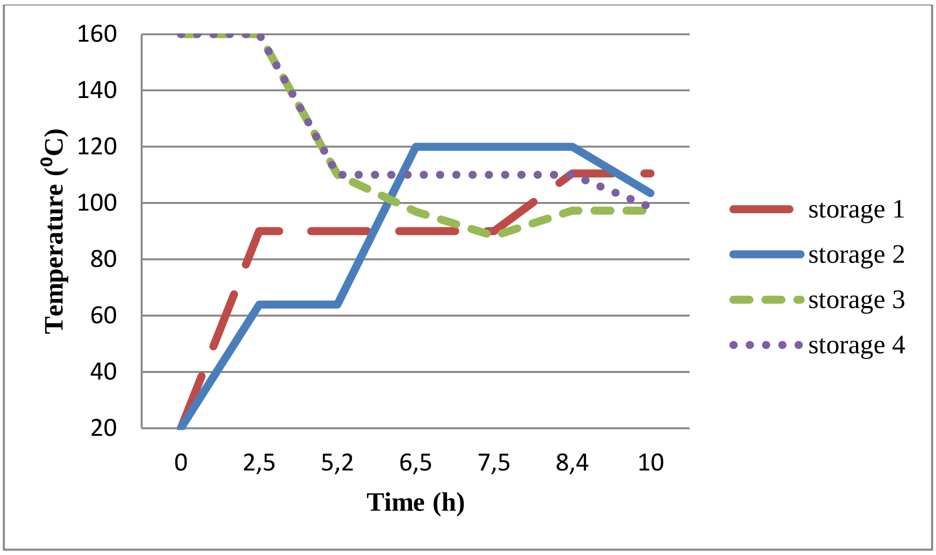


Figure 4.13: Temperature profile of heat storage vessels for second illustrative example

4.4. Appendix A

The scheduling data for the first illustrative example is given in Table 4.3. The table shows each task with the corresponding maximum batch size and the residence time.

Table 4.3: Scheduling data for first illustrative example

Task	Unit	Max batch size (kg)	Residence time, τ (hr)
Reaction	R1	60	2
	R2	60	2
Filtration	F1	80	1
	F2	80	1
Distillation	D	140	2

Additional scheduling data is given in Table 4.4. This table shows each state with the corresponding initial inventory values, maximum storage and the revenue or cost of each state. As previously mentioned, the cost of raw materials is assumed to be 0.

Table 4.4: Scheduling data for first illustrative example

State	Material state	Initial inventory (kg)	Max storage (kg)	Revenue or cost (c.u)
S1	Feed A	1000	1000	0
S2	Feed B	1000	1000	0
S3	IntAB	0	50	0
S4	IntBC	0	50	0
S5	Waste	0	1000	0
S6	Prod 1	0	1000	120
S7	Prod 2	0	1000	120
	Cold utility			0.02
	Hot utility			1

The heat integration data is given in Table 4.5. This table gives the supply and target temperatures for each task as well as the specific heat capacities.

Table 4.5: Heat integration data for first illustrative example

Task	Supply temp, $T^s(s_{inj})$ (^{0}C)	Target temp, $T^t(s_{inj})$ (^{0}C)	Unit	Specific heat, $cp(s_{inj})$ (kJ/kg^{0}C)
Reaction	100	70	R1, R2	3.5
Distillation	65	80	D	2.6

The heat storage vessels cost function parameters are given in Table 4.6. These parameters are the fixed cost, variable cost, operational time, cost function exponent and the number of years a heat storage vessel can be used.

Table 4.6: Heat storage vessel cost function parameters

Parameter	Symbol	Value
Fixed cost	α_{sto} (c.u)	48 000
Variable time	β_{sto} (c.u/kg)	280 000
Operational time	hr/yr	7920
Cost function exponent	θ	0.6
Interest rate	a (%)	15
Number of years	n (yr)	3

The scheduling data for the first illustrative example is given in Table 4.7. The table shows each task with the corresponding maximum batch size and the residence time.

Table 4.7: Scheduling data for second illustrative example

Task	Unit	Max batch size (kg)	Fixed time α (hr)	Variable time β (x10^{-3}) (hr/kg)
Heating	1	100	0.667	6.67
Reaction1	2	50	1.334	26.64
	3	80	1.334	16.65
Reaction2	2	50	1.334	26.64
	3	80	1.334	16.65
Reaction3	2	50	0.667	13.32
	3	80	0.667	8.33
Separation	4	200	1.3342	6.66

Additional scheduling data is given in Table 4.8. This table shows each state with the corresponding initial inventory values, maximum storage and the revenue or cost of each state. As previously mentioned, the cost of raw materials is assumed to be 0.

Table 4.8: Scheduling data for second illustrative example

State	Material state	Initial inventory (kg)	Max storage (kg)	Revenue or cost (c.u)
S1	Feed A	1000	1000	0
S2	Feed B	1000	1000	0
S3,S4	Feed C	1000	1000	0
S5	HotA	0	100	0
S6	IntAB	0	200	0
S8	IntBC	0	150	0
S9	ImpureE	0	200	0
S7	Prod1	0	1000	20
S10	Prod2	0	1000	20
	Cold utility			0.02
	Hot utility			1

The heat integration data is given in Table 4.9. This table gives the supply and target temperatures for each task as well as the specific heat capacities.

Table 4.9: Heat integration data for second illustrative example

Task	Supply temp, $T^s(s_{inj})$ (^{0}C)	Target temp, $T^t(s_{inj})$ (^{0}C)	Unit	Specific heat, $cp(s_{inj})$ (kJ/kg^{0}C)
Reaction 1	100	70	2, 3	3.5
Reaction 2	70	100	2, 3	3.2
Reaction 3	130	100	2, 3	2.6

The heat storage vessels cost function parameters are given in Table 4.10. These parameters are the fixed cost, variable cost, operational time, cost function exponent and the number of years a heat storage vessel can be used.

Table 4.10: Heat storage vessels cost function parameters

Parameter	Symbol	Value
Fixed cost	α_{sto} (c.u)	48 000
Variable time	β_{sto} (c.u/kg)	280 000
Operational time	hr / yr	7920
Cost function exponent	θ	0.6
Interest rate	a (%)	15
Number of years	n (yr)	3

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CHAPTER 5

RECOMMENDATIONS AND CONSIDERATIONS

5.1. Introduction

Recommendations and considerations are discussed in chapter 5. The recommendations outlined include the transformation of bilinear and trilinear terms in the proposed formulation. The way in which the computation time of the model can be reduced is also discussed. There are also considerations for future work detailed in chapter 5.

5.2. Recommendations

The mathematical model presented resulted in a mixed integer nonlinear programming model. This is due to trilinear terms present in some constraints such as the heat constraints which describe the amount of heat transferred to and from the storage. Constraints (1) and (2) are given as follows:

$$Q_c\left(s_{jc}^{in},v,p\right)=W(v)c_p^w\left(T^i(v,p)-T^f(v,p)\right)z\left(s_{jc}^{in},v,p\right) \qquad \forall s_{jc}^{in}\in S_{jc}^{in},p\in P \tag{1}$$

$$Q_h(s_{jh}^{in},v,p)=W(v)c_p^w\left(T^f(v,p)-T^i(v,p)\right)z\left(s_{jh}^{in},v,p\right) \qquad \forall s_{jh}^{in}\in S_{jh}^{in},p\in P \tag{2}$$

The trilinear terms are created by the multiplication of a binary variable with two continuous variables. This resulted in large computational times where an upper bound for the CPU time had to be set. The results obtained from the model do not result in globally optimality, which for mixed integer non-linear programming models can be achieved by transforming the nonconvex model to a convex model. According to Lundell & Westerlund (2012), convex models are guaranteed optimality while nonconvex models are not guaranteed such optimality. The transformation of an MINLP model to MILP (convex) model can be achieved by implementing Glover transformations or Reformulation-Linearisation. These transformations and the structure of the MILP solutions need to be considered in order to reduce the computational time of the model.

5.2.1. Linearisation of mixed integer non-linear programming models

In order for the computational time for MINLP models to be reduced, linearisation techniques can be implemented in order to reduce the non- linearity and the complexity of the models. There are exact and inexact linearisation techniques. Exact linearisation techniques are those that resultant linearised model is still the same in terms of the constraints and the bounds placed on the variables. The inexact formulation is that when the new constraints introduced may violate the initial constraints and bounds of the model. The following two linearisation methods were considered as linearisation techniques, these are the Glover transformation technique as well as the reformulation linearization technique.

a) Glover Transformation

Glover transformations were presented by Glover (1975) as a method to linearise bilinear terms resulting from the multiplication of a continuous variable and a binary variable. Consider constraint 3 where x is the binary variable and y is the continuous variable. Glover transformation variable is introduced as Γ.

$$xy = \Gamma \tag{3}$$

The lower and upper bounds of the continuous variable are expressed in constraint 4, as would be should y not be multiplied with a binary variable. In order to represent the bilinear term with the glover transformation variable, the binary variable x is multiplied to y as shown in constraint 5.

$$y^L \le y \le y^U \tag{4}$$

$$y^L x \le \Gamma \le y^U x \tag{5}$$

The final formulation of the glover transformation after multiplying by $1-x$ is given as constraint 6.

$$y - y^U(1-x) \le \Gamma \le y + y^L(1-x) \tag{6}$$

b) Reformulation Linearisation technique

The technique was presented by (Sherali & Alameddine, (1992), as discussed by (Quesada & Grossmann (1995). This method is an inexact linearisation method that introduces bounds on the variables which may result in an extended search space to the bilinear terms. Constraint 7 describes the bilinear linear term as a product of a new variable Ψ .

$$ab = \Psi \tag{7}$$

The upper and lower bound for continuous variables a and b are given in constraints (8) and (9).

$$a^L \leq a \leq a^U \tag{8}$$

$$b^L \leq b \leq b^U \tag{9}$$

The search space is then extended by boundary constraints (10), (11), (12) and (13).

$$\Psi \geq a^L b + b^L a - a^L b^L \tag{10}$$

$$\Psi \geq a^U b + b^U a - a^U b^U \tag{11}$$

$$\Psi \leq a^U b + b^L a - a^U b^L \tag{12}$$

$$\Psi \leq a^L b + b^U a - a^L b^U \tag{13}$$

The reformulation linearisation method does not guarantee optimality and therefore the solution obtained after linearisation is used as starting values for the MINLP. If the objective of the MILP is equal to that of the MINLP, then the solution is a globally optimal solution and if the objective of the MILP and the MINLP is not equal, then the solution is a local optimum. The flow diagram of the reformulation linearization is given in Figure 5.1.

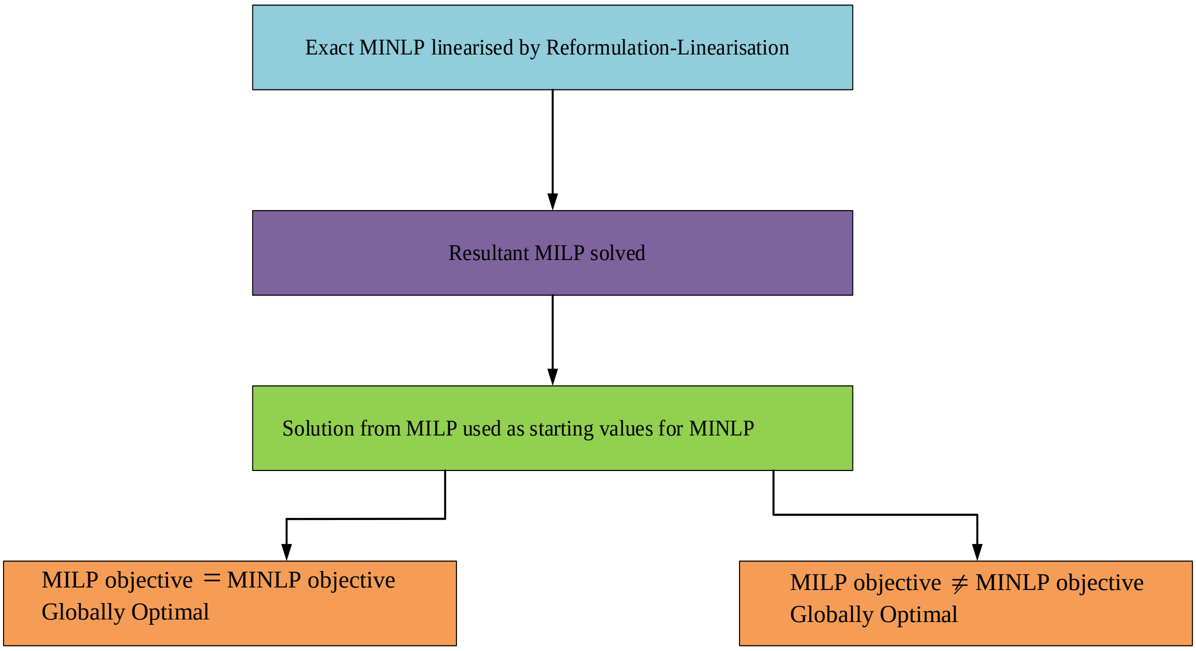

Figure 5.2: Reformulation-linearisation technique

5.2.2. Solution of MILP models

Modelling realistic problems often leads to large scale mixed integer linear programming models which affect the computational efficiency for the solution of the MILP model. Several approaches have been used to exploit certain special structures of specific problems which can be used to override the problem of computational efficiency (Floudas & Lin, 2005).

a) Reformation

Reformulation is used when constraints which have been written in a certain way, are changed and reformulated to a different structure. The aim of this is to tighten the integrality gap, reduce the number of binary variables and have structures that facilitate the solution.

b) Addition of cut constraints

The addition of constraints to an MILP problem may cut off infeasible solutions at an early stage of the branch and bound searching process and therefore can result in a reduced solution time. This can be done through generating special structures or existing insights on the physical problem.

c) Use of heuristics

Heuristics is use of experience to learn and improve on a particular solution can be used to decrease the computational efficiency of a model. The use of heuristics does not guarantee optimality but has been used by researchers such as Pinto and Grossmann (1995) and Blomer and Gunther (2000).

d) Decomposition

Decomposition is when a larger complex problem is divided into smaller sub-problems which can be solved much more efficiently. It should be noted that the decomposition approaches lead to suboptimal solutions but they reduce the complexity of the problem and the solution time.

5.3. Considerations for Future work

In order for the model to be more robust in the future, there are a few considerations that need to be taken into account. This is outlined below and includes the consideration of the initial input of the number of storage vessels, the design of the entire plant, the inclusion of many-to-one connections of the heat storage to different tasks as well as heat losses of the storage vessels.

5.3.1. Input number if storage vessels

The model is structured in such a way that there needs to be an input number of storage vessels and the model will then find the optimal number of heat storage vessels. This can be a very broad task because there is currently no indication of how the initial number of heat storage vessels can be estimated. The higher the initial estimate of the heat storage vessels, the more computational intense the model becomes due to the presence of additional trilinear terms. A method can then be developed where the initial number of heat storage vessels can be determined that can be close to the optimal number of heat storage vessels and therefore decreasing he computational time necessary to obtain the solution to a specific problem.

5.3.2. Design of entire batch plant

The proposed mathematical formulation focuses on the design of the heat storage vessels. This can further be extended to the design of the entire batch plant which will take into account the scheduling of the batch plant as well as the energy minimisation of the plant. This can be achieved by looking at the cost of vessels, reactors and other equipment, as well as cost of energy minimisation while maximising the throughput of the plant.

5.3.3. Many-to-one connections of the heat storage vessel

In the formulation proposed, a heat storage vessel can only be integrated with one task at a specific time point, shown in Figure 5.2. This was given as a practicality constraint in order to facilitate ease in production and heating/cooling in the plant. This constraint can be extended in order to include many to one connections of a heat storage vessel at a certain time point. Considerations of piping connections can also be taken into account in order to account for the connections in a more practical manner.

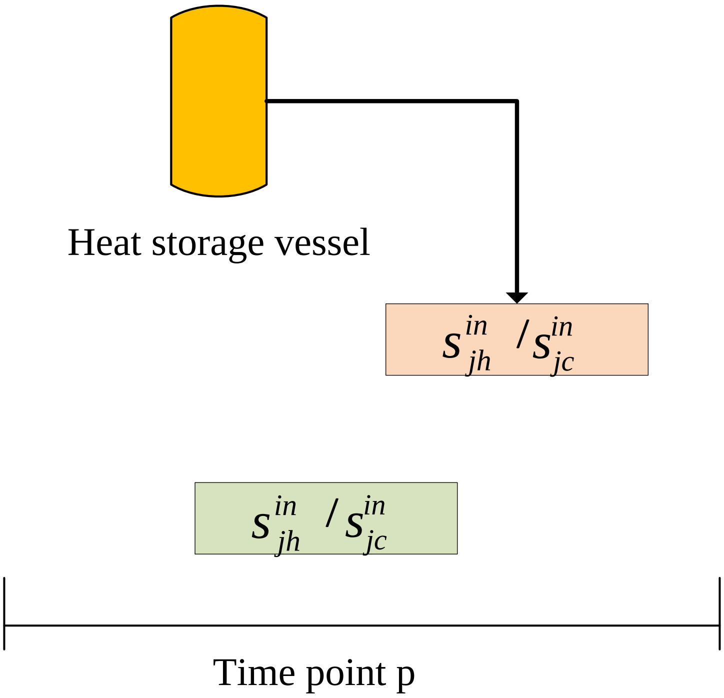

Figure 5.3: One-to-one heat storage vessel connection

5.3.4. Considerations of heat losses

Heat losses can be taken into account in formulation. For the proposed formulation, heat losses were not considered because of the short time scheduling is being considered, the time horizon are short and therefore the idle time of heat storage vessels be short. This results very little heat being lost to the environment when the heat storage vessels are ideal and therefore the inclusion of heat losses do not affect the solutions obtained from the problems.

5.4. References

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CHAPTER 6

CONCLUSION

A mathematical formulation for direct and indirect heat integration with multiple heat storage vessels has been developed and applied to two illustrative examples. The emphasis of the formulation is the use of multiple heat storage vessels by looking at the design of the heat storage vessels as well as the synthesis of the heat exchanger network of the batch process. The proposed formulation uses a continuous time model and has opportunities for FIS operational philosophy. The formulation is aimed at maximising profit in the plant while taking into account the utility and capital costs of the heat storage vessels as well as determining the size and initial temperatures of the heat storage vessels. The proposed formulation resulted in a MINLP formulation due to the presence or trilinear terms.

The application of the formulation results in an increase in profit and the elimination of external utilities use in the plant. The first illustrative example resulted in a 100% decrease of external utilities and an 8.88% increase in profit was obtained when multiple heat storage vessels were considered as compared to when no heat integration is applied to the illustrative example. The second illustrative example resulted in a 100% decrease in external utilities as well as a 17.74% increase in profit when multiple heat storage vessels were considered as compared to a scenario where only one heat storage vessel is available in the plant. The total reduction in external utilities used in both examples does not include the hot and cold utilities used in the heat storage vessels as heat transfer mediums which are already available at the beginning of the time horizon. The use of multiple heat storage vessels showed a resultant flexibility in time which maximised the throughput of the plant while minimising the operational costs of the plant.