Process Scheduling and Heat Integration of Multipurpose Batch Plants using Three Index Unit-Specific Event Based Models

Submitted in partial fulfillment of the requirements for the award of the degree of

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CERTIFICATE

This is to certify that the thesis entitled "**Process Scheduling and Heat Integration of Multipurpose Batch Plants using Three Index Unit-Specific Event Based Models"** being submitted by **Mr. M. SEMAL SEKHAR (Roll No.715064)** for the award of the degree of Doctor of Philosophy (Ph.D) in Chemical Engineering to the National Institute of Technology, Warangal, India is a record of the bonafide research work carried out by him under my supervision. The thesis has fulfilled the requirements according to the regulations of this Institute and in my opinion has reached the standards for submission. The results embodied in the thesis have not been submitted to any other University or Institute for the award of any degree or diploma.

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DECLARATION

This is to certify that the work presented in the thesis entitled " **Process Scheduling and Heat Integration of Multipurpose Batch Plants using Three Index Unit-Specific Event Based Models**" is a bonafide work done by me under the supervision of **Dr. V. Ramsagar** and was not submitted elsewhere for award of any degree.

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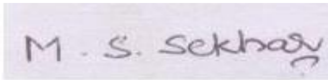

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M. SEMAL SEKHAR

Abstract

Over the past few decades, process scheduling received significant attention in most of the industries involving complex processes to achieve goals such as maximization of profit and minimization of makespan with efficient usage of limited resources available. Batch processes in most of the chemical industries are complex in nature. Industries involved with unit operations such as distillation, drying and evaporation are highly energy intensive. Therefore energy savings in batch processing facilities plays a vital role. Process scheduling coupled with heat integration has been a promising intensification methodology for energy conservation. Researchers in the past had developed several models based on discrete and continuous time frameworks to solve simultaneous short term/cyclic scheduling and heat integration problems. However, the advantages of unit-specific event-based (USEB) modelling approach are not extensively explored.

To fill this research gap, the present study is carried out in four parts. Firstly, a three index unit specific event based (USEB) model is proposed for the simultaneous short-term scheduling and direct heat integration of batch plants. A mixed integer linear programming (MILP) model is formulated which can be used to solve both the standalone and heat-integrated batch scheduling problems. The major emphasis is on the inclusion of novel model equations to improve model statistics and computational performance compared to the existing models available in the literature. The performance of the proposed model is evaluated by considering two benchmark examples. Secondly, a novel unified three index unit-specific event-based mathematical formulation is presented for cyclic scheduling of multipurpose batch plants. The unified framework reduces to a simple case in the absence of cyclic scheduling. The task extending to the next cycle is integrated with the short term scheduling constraints using the active task concept. Further, the framework is also extended for simultaneous cyclic scheduling and direct heat integration of multipurpose batch plants. The computational performance of the unified framework is evaluated with benchmark examples taken from the literature. Thirdly, a robust unit-specific event-based framework is proposed for short term scheduling and indirect heat integration. Using the concept of active task, various modelling issues such as task alignments, energy balances, direct and indirect heat integrations have been handled precisely with minimum number of equations and variables. The effect of the amount of thermal fluid, initial temperature and number of storage vessels on profit is systematically analyzed. The accuracy of the proposed framework is demonstrated using three benchmark examples. The proposed model could effectively incorporate the direct and indirect heat integration and external utility usage. The computational results show that this integration finds an optimum number of heat storage vessels and outperforms the other recent models presented in the literature. Finally, a rigorous Unit Specific Event Based model (USEB) is proposed for optimal utilization of direct and heat integration possibilities in long term scheduling of batch processes. The proposed approach addresses the complete scheduling of long-term operational horizon by considering start-up, cycle and finishing periods. The start-up period takes care of intermediate material states requirement at the beginning of first cycle and finishing period effectively utilizes the leftover intermediate states at the end of final cycle. Using the cyclic scheduling concept, different features of direct and indirect heat integration possibilities are accurately modelled by considering design and optimization of heat storage vessels. The comprehensive computational approach presented in this work highlights the importance of judicious use of direct and indirect heat integration in process industries and cyclic scheduling for complex and long term scheduling problems.

Keywords: Unit specific event based model, Multipurpose batch plants, Cyclic scheduling, Heat integration, Active task, Unified framework, MILP, MINLP, Design and optimization of heat storage vessels.

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CHAPTER 1

INTRODUCTION

Introduction

Chemical processes can be broadly classified into batch and continuous processes. In batch plants, raw materials are converted into final products by a set of discrete processing tasks in a predetermined order (Stamp and Majozi (2017)). Generally, this predetermined sequence is known as a recipe. In batch process, the operating conditions vary with time resulting in unsteady state operations, whereas continuous processes have constant inlet and outlet material flow rates and operate under steady state. The discreteness of batch processing task comprises of a series of events such as feed addition, processing and product removal, as illustrated in Fig. 1.1(a). In continuous process these events happens simultaneously as described in Fig. 1.1(b). The continuous processes have following advantages: bulk production, uniform output quality, easy controllability and handling of materials. Batch plants are preferred over continuous plants for the production with low throughputs. In general, batch plants have an inherent operational flexibility to adapt the changes in product specifications (Lee et al., 2015). Different process recipes can be handled in common equipment whose operating conditions can be modified to allow different range of products. Therefore, even today batch processes are widely used for production in different industries such as pharmaceutical, fine chemicals, polymers, food and explosives. Moreover, batch processes provide flexibility for handling of periodic and fluctuating demands.

Batch processes scheduling has been extensively used to develop objective oriented operational schedules by effectively utilizing the available limited common resources. Batch processes have attracted interest from both industry and academia due to the following unique positive characteristics (Fernandez et al., 2012): i) the manufacturing operations are independently carried out in batches ii) sharing of resources (cooling water, steam, equipment, electricity, etc.) iii) flexibility (connect the equipment in different ways) iv) multipurpose equipment (for instance, an equipment may be used as a storage unit or as a processing unit).

Batch plants are classified into multi-product and multipurpose batch plants depending on the materials flow through the processing equipment (Sparrow et al., 1975). In multiproduct plants, all the products follow the same operational path and use the same equipment. In these plants, usually, only one product can be manufactured at a time. Multipurpose batch plants allow the production of products using different equipment sequences and in some cases two or more products can be produced simultaneously. Multiproduct plants are a subset of multipurpose plants. Multipurpose plants are more flexible in handling different products but they have complex configurations compared to multiproduct plants. Throughput of multipurpose batch plants can be enhanced significantly by effective utilization of the shared resources. Therefore, batch process scheduling can be an effective technique to increase the usability of batch plants.

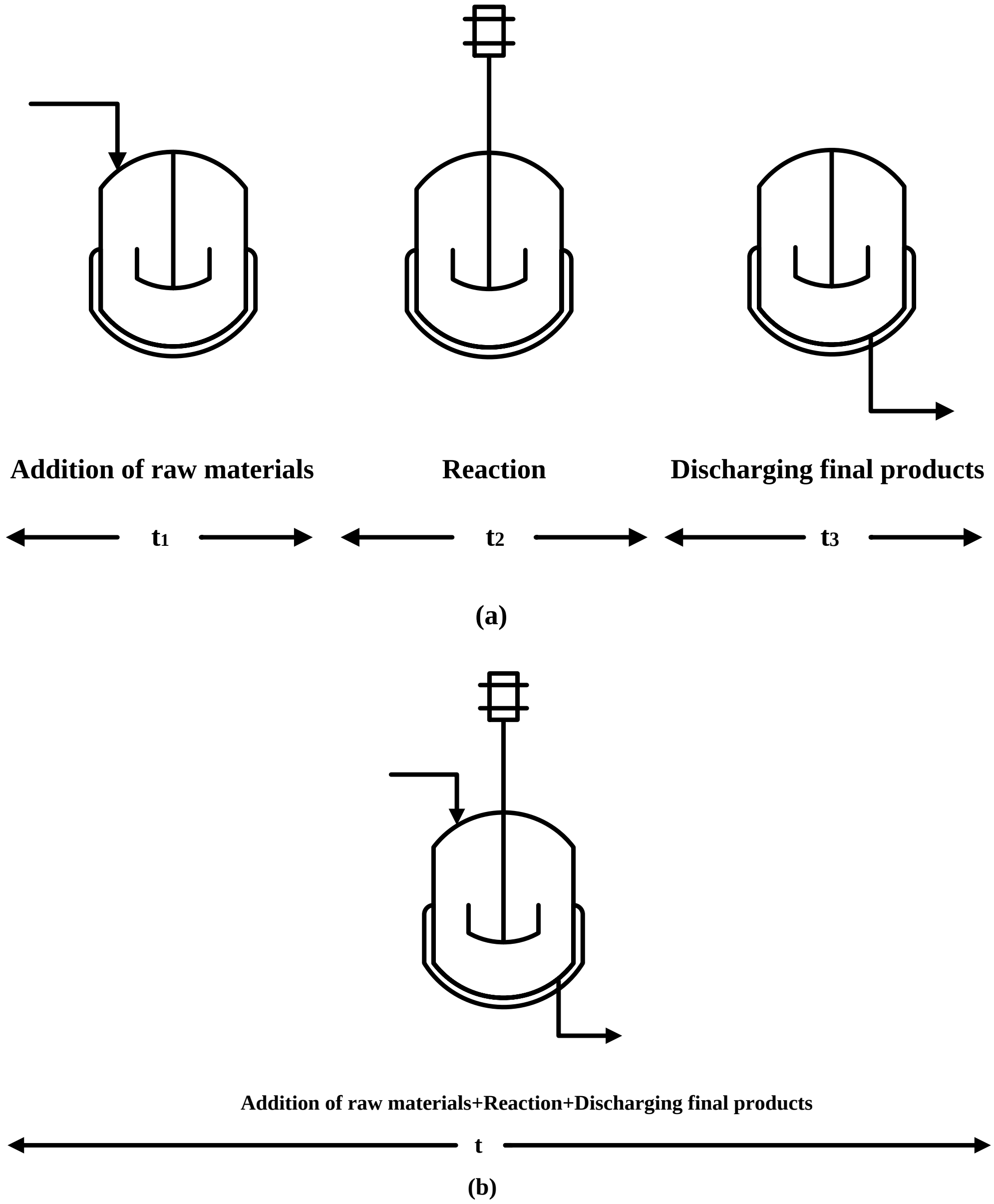


Fig. 1.1. (a) Batch reactor (b) continuous reactor (Majozi, 2010)

Different scheduling aspects including storage policies, material transfer times, variable production and consumption, resource allocation, unit wait times and cyclic scheduling are well studied using different mathematical models (Harjunkoski et al., 2014). Further, the scope of a scheduling problem has been expanding by involving complex features such as heat integration, pipeline scheduling, crude oil and refined products blending, batch versus continuous blending (Castro et al., 2018). Among these options, simultaneous scheduling and heat integration is attracting attention in recent times, because this is a promising intensification technique for energy conservation in chemical industries. This methodology can help in the reduction of CO_2 emissions by designing sustainable industrial process schedules. Consequently, the main emphasis of this work is on the development of novel mathematical models to address some of the current challenges in the field of simultaneous scheduling and heat integration.

The rest of this chapter is organized as follows, Section 1.1 describes the different operational philosophies of batch processes. Section 1.2 presents the insights of batch process scheduling, heat integration and cycling scheduling. An overview on different process scheduling modelling approaches is presented in section 1.3. The motivation behind the proposed research is highlighted in section 1.4. At the end, a broad outline and organization of the thesis is presented in section 1.5.

1.1 . Operational philosophies of batch processes

Depending on the material states storage properties and available capacities, the following different batch process operational philosophies are derived (Pattinson and Majozi (2010)).

Zero wait (ZW): The intermediate materials which need to be consumed as and when they are produced are referred to as zero wait materials. Thus, the zero wait material states need to be transferred to the consumption processing unit immediately after their production. The consumption task must start immediately after receiving the zero wait material state. The ZW policy is used for unstable products, where delay in processing may change the physical and chemical properties of that material.

No intermediate storage (NIS): In this policy, the intermediate material state will not have separate storage unit, however it can stay in equipment unit after processing. The intermediate material state can also be transferred to another processing unit and wait in that unit till the consumption task starts.

Finite intermediate storage (FIS): This policy is more representative of batch operations where there is an existence of storage vessels with finite capacity. This policy is further classified into dedicated finite intermediate storage (DFIS) and shared finite intermediate storage (SFIS). In DFIS policy, each intermediate material state will have at least one dedicated storage vessel. In SFIS policy, a storage vessel can be used to store different material states, however only one material is allowed to store at any time point.

Unlimited intermediate storage (UIS): It is more of a realistic operational policy used in design of batch plants. Large storage capacity can be facilitated to ensure unrestricted production of intermediate material state.

Mixed intermediate storage (MIS): This policy is found in a situation where at least two of the operating policies FIS, NIS, UIS and ZW coexist in a single method.

1.2. Introduction to batch process scheduling, cyclic scheduling and heat integration

A well-defined production schedule is essential in order to achieve high productivity and economic efficiency in batch processes by effective utilization of available resources and operational time. A production schedule can be generated by considering two different objective functions: minimization of makespan and maximization of profit. In makespan minimization the emphasis is on the meeting of a specified product requirement in a minimum time horizon. The aim of profit maximization is to produce the maximum amount of final products in a specified time horizon. These objective functions are often combined with other auxiliary targets such as minimization of utility consumption, unit idle times, changeovers, etc. The increase in demand and popularity of batch plants and striving efforts to reduce the energy utilization laid a strong foundation to the development of novel modeling techniques for batch process scheduling and heat integration. Simultaneous scheduling and heat integration is an interactive approach which can play a potential role in design of energy efficient production schedules.

1.2.1. Batch process scheduling

Scheduling is a decision making process which helps in efficient use of available resources to produce a value-added product. Scheduling plays a predominant role in addressing the factors such as energy efficiency, profit maximization, efficient use of available resources and cost minimization by subsiding the losses and unit idle times (Floudas and Lin (2004); Mendez et al., (2006)). These objectives can be realized by finding the optimal processing time, selection of process equipment and storage vessels, amount of material to be processed or stored (lot-sizing / batching), unit sequencing, task durations, raw material availability, variable mixing and splitting.

The production schedules can be either offline or online. Offline schedules are often used to determine the layout of manufacturing facilities for the products with stable market demand in a long term scenario. While designing the offline schedules, it is more important to find optimal solutions than to achieve computational performance. Online schedules are preferred over offline schedules in handling of scheduling under uncertainty (Harjunkoski et al., 2014). Based on the time horizon is considered, the scheduling in general is classified into three categories: (a) long-term scheduling which is dealt relatively using the time horizon in the order of months, (b) medium term scheduling which is carried with the time horizon in the order of weeks and (c) short term scheduling with the time horizon in the order of hours. Decomposition algorithms and stochastic modelling techniques are more effective than the deterministic modelling approaches for handling of long-term and medium-term scheduling problems, which generally have a large problem size. Cyclic scheduling is also a potential alternative for handling of long-term scheduling problems. Deterministic models can effectively handle the short term scheduling of batch plants. Rigorous and robust deterministic mathematical models based on continuous time and discrete time approaches have been developed for addressing different operational features of short-term scheduling.

1.2.2. Heat Integration

Most of the chemical operations need to be carried out at specified operating conditions, in the presence of external heating or cooling. The requirement of external utilities can greatly be reduced by integrating the heat generating process tasks (for example, exothermic reactions) with the tasks require heat (for example, Distillation). Heat integration in general is a system oriented approach incorporated along with process scheduling to obtain an optimal and effective usage of resources (Castro et al., 2015). A large number of chemical industries are highly energy intensive. Heat integration can be carried out in batch plants by exchanging the heat directly or indirectly from hot streams to cold streams. Heat integration is more essential to consummate a stable tradeoff between efficient management of energy resources and minimization of waste. Heat integration for a continuous process has an advantage over a batch process as all the heat integration techniques applied assume time invariant behavior, which is a key feature of any continuous process. Heat integration has less effect on batch process scheduling, when external heat sources and sinks are very cheap and usually available throughout the schedule (Fernandez et al., 2012).

Direct heat integration: In direct heat integration, the hot and cold streams pass through a heat exchanger for exchanging the heat. In the direct heat integration, both hot and cold tasks are integrated only if they are active at the same time interval. The direct heat exchange sometimes enforces tight scheduling conditions to align the heat integrated tasks.

Indirect heat integration: In indirect heat integration, the hot stream energy is transferred to the cold stream by making use of an intermediate stream. Initially, heat is transferred to a thermal fluid from hot process stream, later this heat is transferred to the active cold process stream at different time interval. This approach provides plenty of operational flexibilities by allowing heat exchange between non-coexistent process streams on a real time axis.

Heat exchange using thermal fluid can eliminate or reduce the external hot and cold utility requirements significantly, enhance the overall process energy efficiency and reliability. The two stage heat exchange between the process streams i.e. form hot stream to thermal fluid and from thermal fluid to cold stream requires more number of heat exchangers and high heat exchanger area due to low temperature driving force and more heat load. Further, the total investment costs related to manufacturing heat storage equipment and associated auxiliary equipment like pipes, bends and pumps need to consider in the profit analysis. Hence, economic analysis considering various key parameters such as batch size, revenue from product and process operating conditions is critical to assess the requirement of heat storage.

In particular, indirect heat storage is not a viable option for short term and low temperature operations. However, in long term operations, perhaps the use of heat storage vessels is an attractive option to explore, because the initial capital investment on indirect heat storage facility can be easily recovered in the form of savings due to less external utility requirement.

Heat exchange configurations: A process can be designed with different heat exchange configurations viz., a) process stream can exchange energy with external utilities, b) heat exchange between the process streams and c) heat exchange between the process stream and thermal fluid. In configurations (b) and (c), the deficit energy demand for standalone and heat integrated tasks can be compensated by using external utilities. Design of these configurations mainly depends on the following two key parameters: availability of resources and driving force for heat exchange.

In these configurations, the task requiring cooling is represented as i_c (cooling task) and the task requiring heating is represented as i_h (heating task). In general, the high or low pressure steam, thermal oils and electrical energy can be used as external hot utilities and cold water and refrigerants are used as cold utilities. In configuration (a), the energy requirement of all processing tasks can be met using external hot and cold utilities. A tradeoff always exists between the amount of product produced and the external utilities required, when the price of the product and cost associated with the external utility required to produce that product are similar. This configuration is highlighted using a production schedule with eight processing tasks as shown in Fig. 1.2(a). The same production schedule presented in Fig. 1.2(a) has been used in the subsequent discussion to highlight the advantage of different heat exchange configurations. In this schedule, the processing tasks *i0*, *i1*, *i4* and *i6* require 100KW, 60KW, 50KW and 50KW of cooling. The processing tasks *i2*, *i3*, *i5* and *i7* require 60KW, 180KW, 100KW and 120KW of heating. For the same production schedule, the configuration (b) allows the direct heat exchange between few process streams. To facilitate direct heat integration, the heating and cooling tasks need to coexist on a real time horizon. Fig. 1.2(b) depicts the energy integration and utilization profile using this configuration. The direct heat integration matches can reduce the external utility requirement, hence energy efficient production schedules can be designed with this configuration as compared to configuration (a).

In configuration (c), the heating and cooling requirements can be met from the following options presented in the preference order: direct heat integration, indirect heat integration and external utilities. Indirect heat integration can be handled using a single heat storage vessel or multiple heat storage vessels. In a process with a single heat storage, at any time interval only one of the processing tasks can integrate with the heat storage vessel and other active processing tasks at the same time duration could meet the energy requirement from direct heat integration and/or external utilities. Using the storage vessel the energy from cooling task can be transferred to a suitable active heating task at different time interval as highlighted in Fig. 1.2(c). By using multiple heat storage vessels heat integration flexibility can be drastically increased due to simultaneous heat exchange. Fig. 1.2(d) highlights the energy utilization profile using two heat storage vessels. The production schedules presented in Fig. 1.2 also highlight the use of external utilities, while meeting deficit energy demand of few heat integrated tasks.

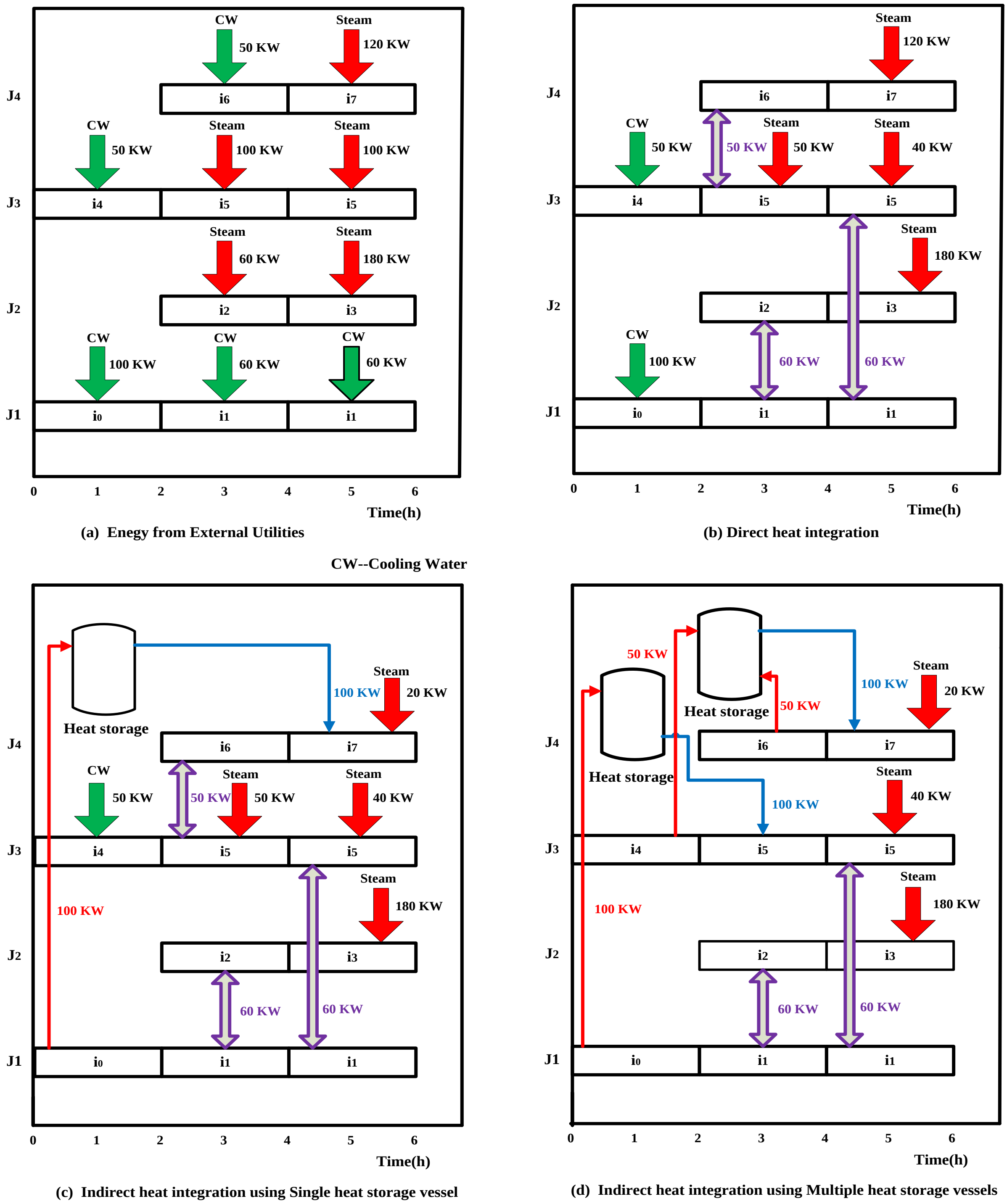


Fig. 1.2. Different heat integration configurations

1.2.3. Cyclic scheduling approach

Scheduling over longer time horizons has limitations such as large problem size, computational complexity, less problem-solving efficiency and accuracy etc. These limitations persuaded researchers to overcome problems associated with scheduling over long time periods. For different industrial cases, the idea of cyclic scheduling of multi-product batch plants using discrete and continuous time representation was proposed. (Shah et al., (1993); Schilling and Pantelides (1999); Wu and Ierapetritou (2004); Castro et al., (2003); Castro and Novais (2007)). In this approach, the long time horizon is divided into cycles of equal time periods in which the task associated with each of the cycles is repeated, which is the basic principle of cyclic scheduling. The splitting up of the long term scheduling problem into sub-schedules with smaller time periods reduces the problem size and helps in achieving a converged solution. This sub schedule can be executed repeatedly over predefined time intervals. Although this decomposition process may not result in the global optimal solution, it is quite effective for solving long term scheduling problems to obtain a near optimal solution. In an independent cycle, the other operational features such as resource utilization, utility integration, storage policies and changeovers can be handled effectively. This kind of approach also helps in improving plant operation by simultaneous implementation of necessary changes that are required to handle process uncertainties and demand fluctuations.

Cyclic scheduling mainly considers the time length of the cycle (unit period) and schedule decisions (unit schedule) as variables in optimization. Each of the unit periods is associated with the tasks taking place within the period and cross over tasks to the next period, as shown in Fig. 1.3(a). To model this unit period, the tasks which are extended to next cycle are notionally wrapped up to the beginning of the cycle as presented in Fig. 1.3(b). At the beginning of the unit period, each unit schedule requires certain amounts of intermediates and these can be produced in previous cycle. For the first unit period, the amounts of intermediates required at the beginning are produced in initial time period. Similarly, the cross over tasks from the last unit period can be accommodated in final time period as shown in Fig. 1.4. At the end, initial and final time periods can be solved as makespan minimization problems for the specified intermediate material states demand by using the unit schedule. Later the initial and final periods can be solved for maximization of profit to increase the productivity.

1.3. Classification of process scheduling models

Numerous mathematical models have been proposed in the literature for addressing different operational aspects of batch process scheduling. These models are mainly characterized as deterministic and stochastic models. The deterministic models are further divided into subgroups based on time representation, event representation and process flow sheet representation. These categories are briefly discussed in the subsequent subsections. For long term and large size scheduling problems the use of stochastic modeling approaches such as Tabu Search (Glover, 1990), Simulated Annealing (Aarts and Korst (1989)), Genetic Algorithms (Goldberg, 1989; Ramteke and Srinivasan (2011); Costa, 2015), or evolutionary techniques (Heinonen and Pettersson (2003)) may be preferable. Since these algorithms can obtain good quality solutions within reasonable time. These approaches decompose the scheduling problem into multiple layers and these layers are solved simultaneously or sequentially using suitable heuristics. These techniques guarantee the solution for complex problems, although it may not be always the optimum. Unlike the stochastic models, in deterministic models no randomness is involved and hence the converged solution always is at global optimum. However, the models may not lead to converged solution while handling large scale problems. Consequently, optimization research community is striving hard to improve the computational performance of deterministic models. In line with the global optimization research community objective, this thesis targets the development of novel and efficient deterministic models to effectively handle some of the current scheduling challenges.

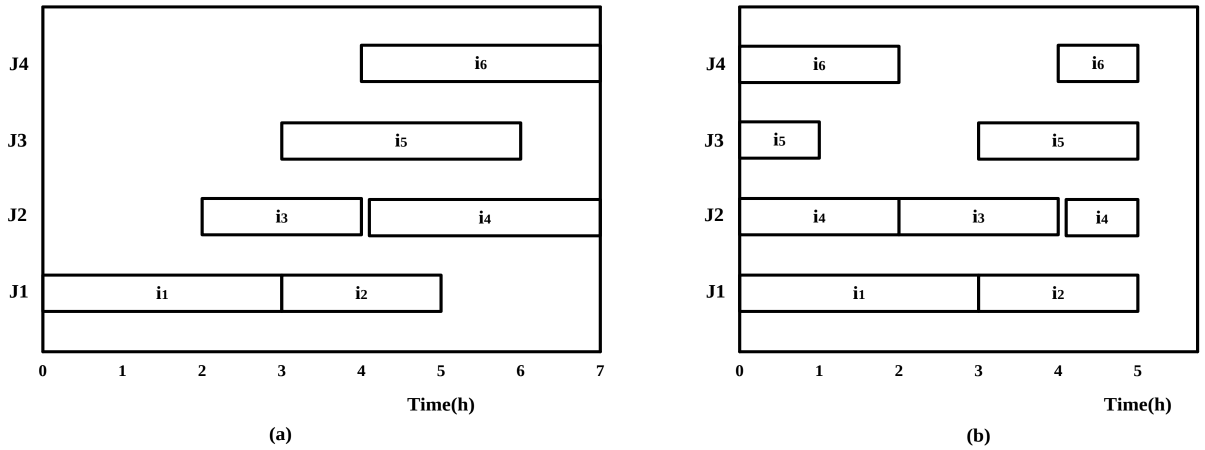


Fig. 1.3. Cyclic Scheduling Gantt chart (a) Unit Schedule with crossovers (b) Equilvalent Unit Schedule

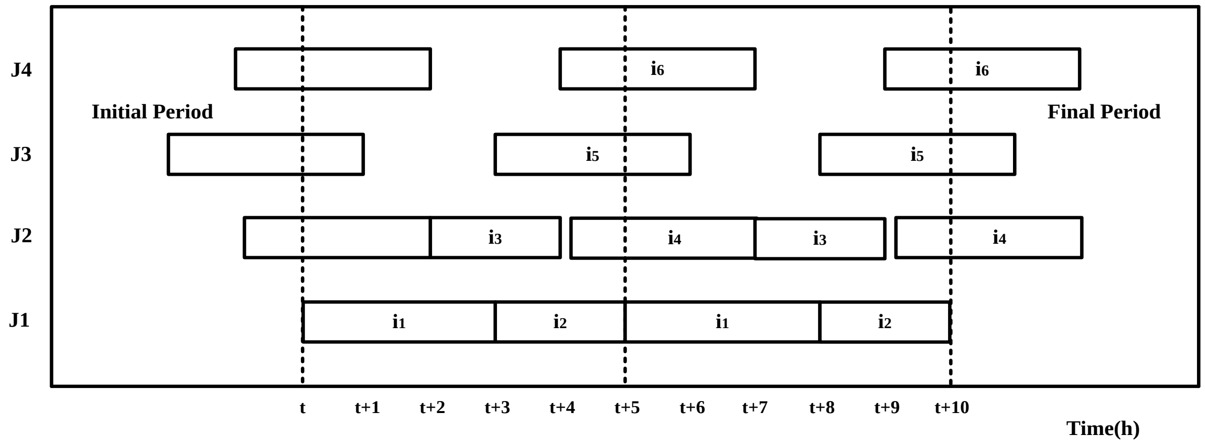


Fig. 1.4. Cyclic Scheduling Gantt chart with initial and final time periods

1.3.1. Time representation

Based on the time representation all the scheduling formulations are mainly divided into two categories viz., discrete time models and continuous time models. Discrete-time models divide the time horizon into a finite number of time intervals with known duration and the instances of task starting and ending are always associated with the boundaries of time intervals (Kondili et al., 1993). The discrete-time models have the main advantage in handling different scheduling aspects using simple mathematical equations, which can be relatively easy to formulate based on the finite time intervals (Floudas and lin(2005); Janak and Floudas (2008)). Due to the above advantage, these models still have an edge in handling some of the complex scheduling features. However, the discrete-time models may fail in handling large scale scheduling problems due to the following limitations: discretization of time intervals which results in accomplishing sub-optimal solutions, requires a large number of binary and continuous variables and significant increase of model size for long time horizon. The drawbacks of discrete-time models mentioned above may create a hindrance in achieving objectives such as maximizing profit and minimizing the cost of production with optimal usage of available resources. Thus, continuous-time models have become a maneuver for researchers to achieve global optimal solutions. Continuous-time models divide the time horizon into a number of time intervals with variable duration. Continuous models are classified into four distinct categories such as slot-based, global event-based, unit-specific event-based (USEB) and precedence based formulations. The advantages of continuous time models are better computational performance, smaller problem size and fewer variables. However as the time domain changes from discrete to continuous, the complexity of model increases.

1.3.2. Event representation

Based on the event representations the scheduling models are classified as global time interval based, global event based, slot based and unit specific event based models. Discrete time models use the global time intervals to represent the events and these time intervals with known duration enforce the tasks to start and end at a particular time. In global event based models, the event points are globally aligned across all equipment units. Starting and/or ending of a task triggers the event point at a same location on a real time horizon across all units (Castro et al., (2001); Maravelias and Grossmann (2003); Castro et al., (2004)). In the slot-based models, slots divided the time horizon into unequal time intervals (Karimi and McDonald(1997); Lamba and Karimi(2002)). The slot-based models can be categorized into two types: process slot-based models (or synchronous) and unit slot-based models (or asynchronous). Process slot based models use the common time grid across all the units

(Sundaramoorthy and Karimi (2005); Liu and Karimi (2007); Susarla et al., (2010)). This synchronous time grid simplifies the handling of shared resources, storage, utilities, etc., since the relative timing of the operations in all units are known. If each unit in the process uses an independent time grid then such slots are referred as unit slots. The asynchronous nature enhances the complexity in predicting the relative timing of the operations for accurate monitoring of resource levels. Table 1.1 presents the advantages and disadvantages of global event based, slot based and unit specific event based models.

Table 1.1. Comparison between different continuous-time models

S.No	Continuous-time models	Advantages	Disadvantages
1.	Global event based model	• Event points are aligned across the units. • Handling resource balance is an easy task. • Can handle sequential and network represented processes	• Problem size is large due to uniform event alignment. • Number of events need to be estimated iteratively. • Critical modelling issues: changeovers, intermediate due dates.
2.	Slot based event model	• Slots represent a set of predefined time intervals with unknown durations • Synchronous slots have similarities with global events and asynchronous slots mimic the unit specific events • Effective for sequential processes	• More number of continuous variables required to align the tasks • Number of slots need to be estimated iteratively. • Critical modelling issues: resource constraints, network represented processes.
3.	Unit-specific time event based model	• Allows the different tasks to start at different times ~~at~~ in the same event across the units • It results in smaller problem size and better computational time.	• Require complex model equations to handle alignments and resource balances. • Number of events need to be estimated iteratively. • Critical modelling issues: Intermediate due dates, sequence dependent changeovers.

Unit-specific event-based models introduced the original concept of even points by allowing different task starting time in different units at the same event point (Ierapetritou and Floudas (1998a), (1998b)). Fig. 1.5 shows the requirement of event points for obtaining the same process schedule using different model formulations. As highlighted in the Fig. 1.5, unit-specific event-based models require fewer events compared to global events and process slot-based models, due to heterogeneous locations of event points (Shaik et al., 2006). Further, better computational performance has been observed while solving most of the scheduling problems (Shaik and Floudas(2009); Susarla et al., (2010); Seid and Majozi(2012)).

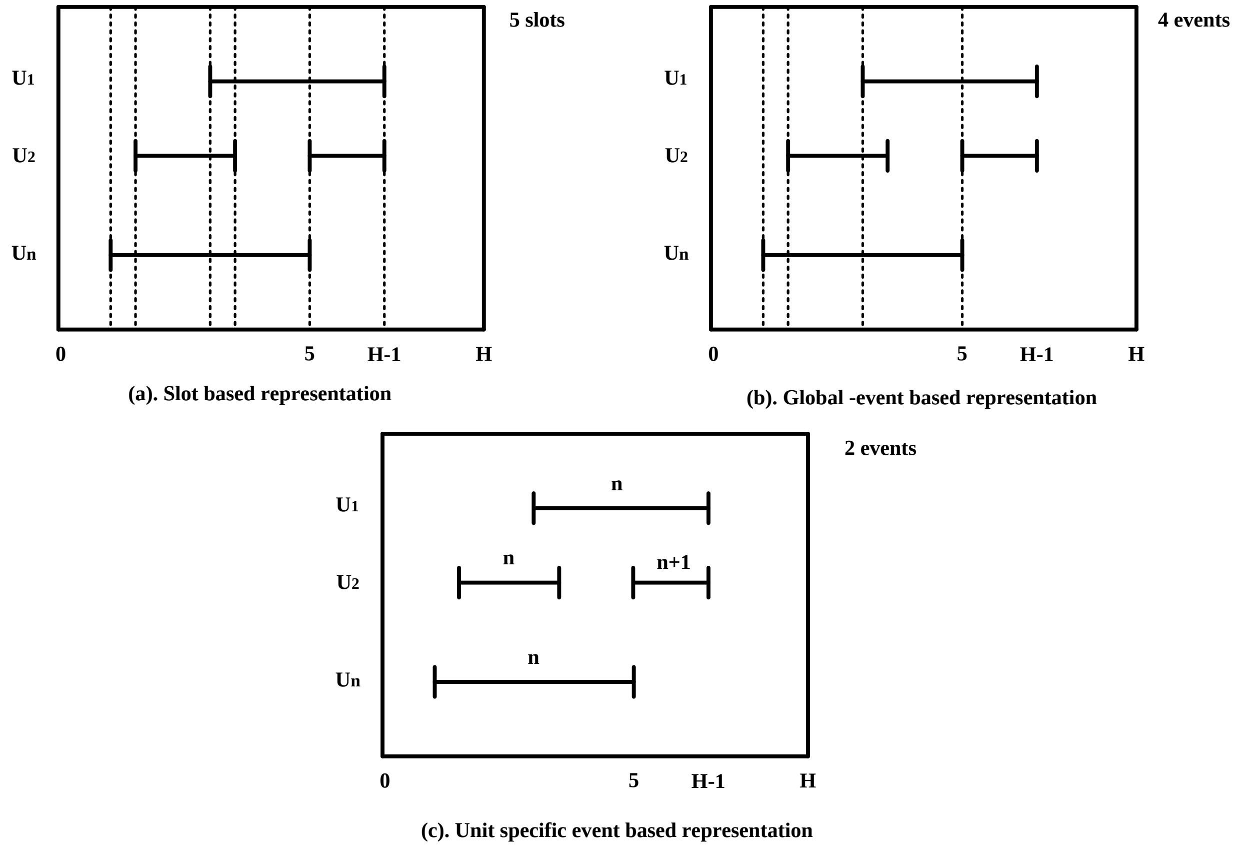
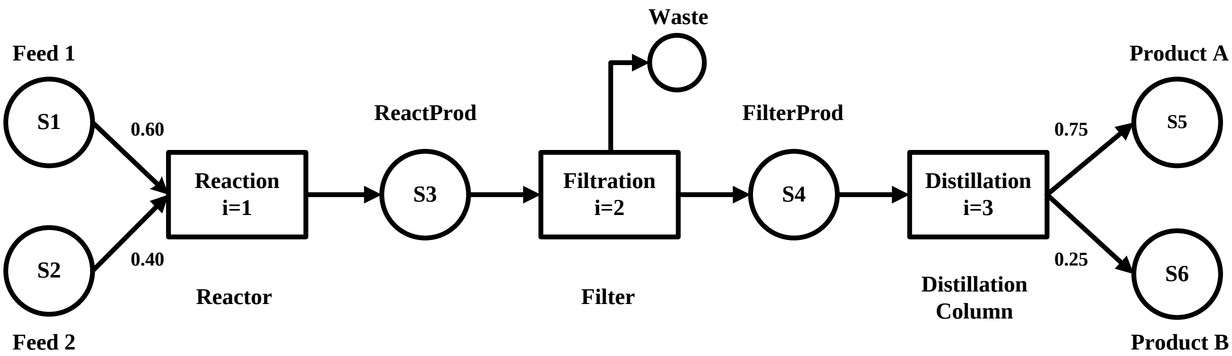


Fig. 1.5. Different continuous-time representations (Sheik et al., 2006)

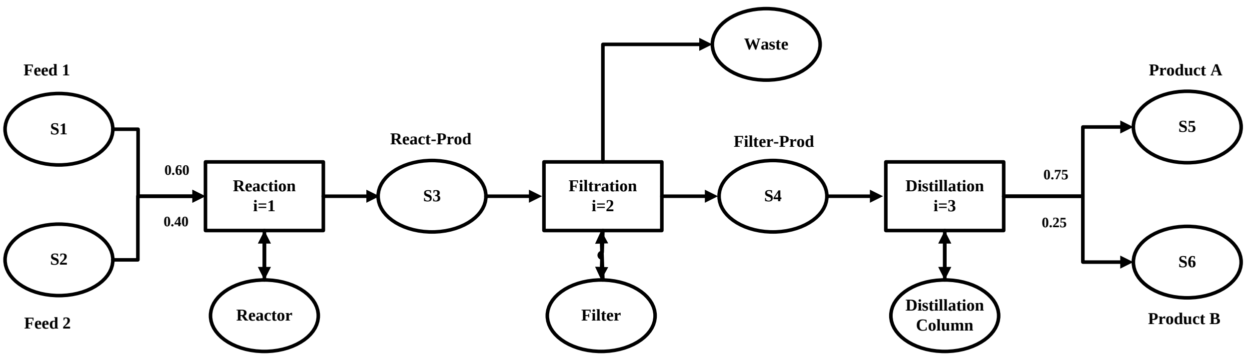
1.3.3. Process flow sheet representation

Based on the process flow configurations the batch processes are categorized into sequential processes and network defined processes. In sequential processes, the same processing sequence is followed by different products. Network represented processes generally have complex features such as recycles, stream splitting and mixing, variable split fraction, etc., and the products will have low recipe similarities (Mendez et al., 2006). In process scheduling jargon, these process flow sheets are presented using state task network (STN), resource task network (RTN) and state sequence network (SSN) representations.

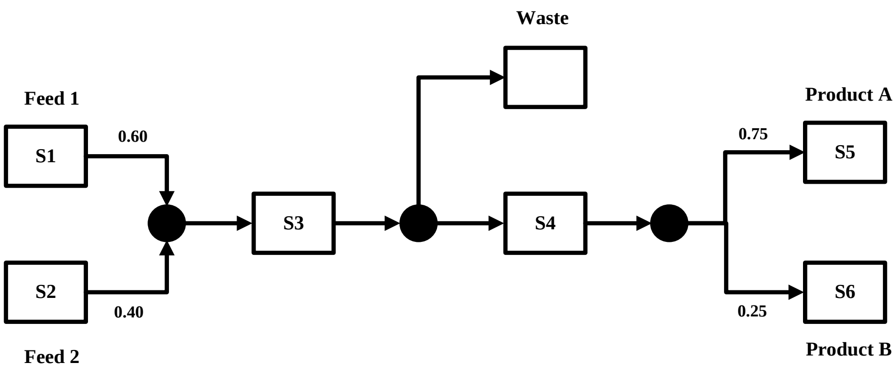
Kondili et al., (1993) first proposed STN flow sheet representation, which mainly consists of following three components (i) state nodes (circle) represent raw materials, intermediates and final products (ii) task nodes (rectangles) depict process operations that convert the material from input states to output states and (iii) arcs that connect states and tasks represent the material flow. Fig. 1.6(a) shows the STN representation of a process consisting of three processing tasks and six material states.



(a). State Task Network (STN)



(b). Resource Task Network (RTN)



(c). State Sequence Network (SSN)

Fig. 1.6. Different process flow sheet representations

Resource task network (RTN) is another common flow sheet representation used in process scheduling and it was first presented in Pantelides (1994). In RTN representation the rectangle denotes the process task which consumes and/or generates multiple resources such as feeds, intermediates, products, manpower, utilities, process equipment and storage tanks, etc. The RTN approach enables the uniform treatment of continuous and discrete resources. Fig. 1.6(b) shows the RTN representation of process flow sheet. Majozi and Zhu (2001) proposed a State Sequence Network (SSN) representation by utilizing the flow of material states. The process tasks are indirectly represented by monitoring change in material properties from stage to stage. Fig. 1.6(c) shows the SSN representation of process flow sheet.

1.4. Motivation behind the proposed research

Numerous modeling approaches are proposed in the literature for short-term scheduling of batch plants. For the last three decades, researchers have been using discrete time and continuous time representations to address a wide variety of scheduling problems. The efficiencies and computational complexities of these models strongly depend on the way of modelling different operational features and the resulting model sizes. For instance, discrete time models may be effective with fixed batch processing times for small-scale problems, whereas continuous time models are considered more effective with fixed / variable batch processing times for larger problems. Further, the model complexity increases as the optimization problem domain increases because of integrating the process scheduling with design, heat integration and control. Therefore, there is a universal concern to establish novel modeling approaches to efficiently manage various complex characteristics of batch operations. Mathematical formulations were also focused on reduction of model size by minimizing the number of events, variables and constraints to enable the optimum solution for large scale processes. However, there is still scope for improvement in the areas in particular to the integration of scheduling with design, heat integration and control.

1.5. Thesis outline

The thesis comprises of seven chapters and a brief outline of each chapter is specified as below.

Chapter 1: This chapter broadly covers the different operational aspects of process scheduling, cyclic scheduling and heat integration of batch plants. Different modeling approaches used for process scheduling and heat integration are systematically reviewed. At the end motivation behind the proposed research is briefly presented.

Chapter 2: In this chapter an up-to-date literature review is presented on simultaneous scheduling and heat integration of batch plants. The review is mainly focused on the evaluation of different unit specific event based models for handling different operational philosophies of batch plants. At the end, the research gaps identified from the literature review are presented along with the proposed objectives of this work, to address these gaps.

Chapter 3: In this chapter a unit-specific event-based model based on STN framework is proposed to handle the short term scheduling of batch plants with and without direct heat integration.

Chapter 4: In this chapter, a novel unified three index unit specific event based model is proposed to handle cyclic scheduling for multipurpose batch plants. Later, direct heat integration policies are incorporated in the proposed model. Computational performance of the unified framework is evaluated with benchmark examples taken from the literature.

Chapter 5: In this chapter, a simplified unit specific event based modeling framework is proposed for direct and indirect heat integration of batch plants with design and optimization of heat storage vessels. The proposed framework explores indirect heat integration in multipurpose batch process scheduling.

Chapter 6: In this chapter, the model proposed in chapter 5 is extended to handle cyclic scheduling of batch plants. Using the active task concept, different features of direct and indirect heat integration of batch plants with design and optimization of heat storage vessels are accurately modelled in cyclic scheduling.

Chapter 7: This chapter highlights the major conclusions drawn from the present work and scope for future work.

CHAPTER 2

LITERATURE SURVEY

Literature Survey

This chapter provides a productive and up to date literature review on short term scheduling, cyclic scheduling and heat integration of batch plants. Different mathematical models available in the literature for simultaneous scheduling and heat integration of batch plants are systematically evaluated. Section 2.1 presents the literature on the short-term scheduling of batch plants with different storage policies and utility resources. Various modeling approaches available in the literature for cyclic scheduling of batch plants are reviewed in Section 2.2. In section 2.3, number of mathematical approaches available in the literature for handling various operational aspects of process scheduling and heat integration are discussed. In section 2.4, the research gaps identified from the literature review are presented along with the proposed objectives to address these gaps.

2.1. Short-term scheduling of batch plants

The advent of scheduling has brought significant attention for addressing operational research problems from the past two decades. Scheduling enables the efficient use of available resources to meet the industrial objectives. The short-term scheduling has received significant attention to resolve problems in different industrial domains by maximizing the profit, minimizing operational cost and efficient use of available resources (Mendez et al., (2006); Floudas and Lin (2004)). The operational time horizon in short-term scheduling is usually limited to hours or days resulting in short response time, minimum uncertainty and high solution feasibility. Deterministic models are extensively used to address different short term scheduling problems. Numerous modelling approaches were proposed to handle process scheduling problems with different operational features such as: storage policies, changeovers, transfer times, utility integration, intermediate demand due dates, etc. Since last two decades, a number of review papers have systematically recorded the major developments along with the future challenges associated with scheduling of batch plants. Table 2.1 shows the insights from some important review papers in this area. In this section the presented literature highlights important contributions on short term scheduling of batch plants with different storage policies and utilities.

Table 2.1. Review papers on process scheduling

S. No	Authors	Title	Description
1.	Kallrath (2002)	Planning and scheduling in the process industry	This article discussed the conceptual thoughts of different planning and scheduling problems, some effective solution approaches to solve these problems and finally concluded with a

			short view on future challenges in process planning and scheduling area.
2.	Floudas and Lin (2004)	Continuous-time versus discrete-time approaches for scheduling of chemical processes: a review	This paper presented a detailed overview of state of the art developments in scheduling of batch and continuous plants. Important characteristics of different discrete-time and continuous-time modelling approaches along with their merits and demerits are discussed. Based on the nature of chemical process and time representation used, the challenges posed to solve the scheduling problem were discussed. Finally, integration of scheduling with design and synthesis of chemical plants and the concept of scheduling under uncertainty was also discussed.
3.	Mendez et al., (2006)	State-of-the-art review of optimization methods for short-term scheduling of batch processes	This article presented a detailed classification of scheduling problems based on different operational aspects such as: process topology, equipment assignment and connectivity, storage policies, material transfers, changeovers, demand patterns, etc. The existing scheduling models in the literature were classified into four groups based on the time representation, material balances, event representation and objective function. The effectiveness and efficiency of different discrete and continuous time models were compared by solving two benchmarking examples from the literature.
4.	Pan et al., (2009)	Continuous-time approaches for short-term scheduling of network batch processes: Small-	This article compared the performance of different continuous time scheduling models based on global events, unit-specific events, process slots and precedence relations. The computational results highlights that the unit specific event based and precedence based

		scale and medium-scale problems	models are effective for handling of short term scheduling problems as they require minimum event points and results into small model size.
5.	Maravelias and Sung (2009)	Integration of production planning and scheduling: Overview, challenges and opportunities	This article highlighted the advantages of integration of production planning and scheduling and also presented effective solution strategies and modeling approaches.
6.	Verderame et al., (2010)	Planning and Scheduling under Uncertainty: A Review Across Multiple Sectors	In this work an overview of the major contributions with specific emphasis on uncertainty analysis within the planning and scheduling area were illustrated. Application of risk minimization techniques such as fuzzy programming, two-stage stochastic programming, chance constraint programming, parametric programming, robust optimization techniques, etc. in different sectors were elaborated.
7.	Harjunkoski et al., (2014)	Scope for industrial applications of production scheduling models and solution methods	This article reviewed the developments in process scheduling area keeping in view scheduling models and methods on industrial applicability. Even though rigorous mathematical models have been proposed to address different operational features of the process scheduling problems, scalability remains a problem as the combinatorial complexity increases as the model extended to solve large scale industrial problems. Hence, the review highlighted the necessity of evolution of optimization methods and algorithms to solve wide variety of industrial problems.

8.	Castro et al., (2018)	Expanding Scope and Computational Challenges in Process Scheduling	In this article, an overview of enterprise-wide optimization and challenges in integration of scheduling with other operational scenarios such as heat integration, pipeline scheduling, refinery components blending, etc. were presented. Recommended the Generalized Disjunctive Programming (GDP) as a new modeling paradigm for solving multiscale scheduling problems as it resulted in better computational statistics than the models used in STN and RTN frameworks.

Grossmann and Sargent (1979) proposed a MINLP based modelling approach to design multiproduct batch plants which results in optimal or near optimal solution. This modelling approach had better computational efficiency than the tedious branch and bound search method proposed by (Sparrow et al., 1975). Suhami and Mah (1982) proposed a MINLP formulation to design multipurpose batch plants. The proposed solution scheme consists of the following stages: feasible sequence generation, each of these sequence was solved using MINLP model by incorporating horizon constraints and selection of optimal or near optimal configurations using heuristic considerations. In the proposed scheme all the selected alternatives were solved using MINLP model which resulted in high computational burden. Vaselenak et al., (1987) introduced a novel formulation for the optimal scheduling and design of multipurpose batch plants where a single MINLP problem based on superstructure concept was solved to get the optimal solution. Different products that can produce simultaneously are embedded as a group using a superstructure and each of these groups were represented by a time period. Birewar and Grossmann (1989) proposed the NLP model for simultaneous design and scheduling of multiproduct batch plants considering unlimited intermediate storage and zero wait policies.

Shah and Pantelides (1992) addressed the design of flexible production multipurpose batch plants considering uncertainty in the production requirements. A multi-period MILP optimization problem was solved where each period represents a scenario with different production requirements. Kondili et al., (1993) proposed a discrete time based MILP formulation for short-term scheduling of batch plants by considering State Task Network (STN) framework for flowsheet representation. The proposed formulation effectively handled the following important features: multipurpose equipment units, variable batch size, mixed intermediate storage policies involving both dedicated and multipurpose storage vessels.

Shah et al., (1993) presented a MILP mathematical model considering the STN framework to address various scheduling problems that arise in multi-product/multipurpose batch facilities. In order to reduce the computational time, some constraints were reformulated to tighten the relaxed MILP solution. The effectiveness of the proposed approach was demonstrated by solving industrial case study on scheduling of hydrolubes plant where different operational scenarios such as finite storage capacity, utility requirements and cleaning requirements were considered.

Pinto and Grossmann (1995) developed an MILP model with continuous time representation using time slots concept for the short-term scheduling of multi-stage batch plants that may involve parallel equipment. Two solution strategies were presented in this formulation. First solution strategy was based on the use of pre-ordering constraints which reduced the problem size significantly. Likewise, the second strategy focused on two stage decomposition techniques where initially task assignments were determined with minimum process time and subsequently the earliness was minimized by solving the LP model. Global event based modelling approach was first explored by Zhang and Sargent (1996) using Resource Task Network (RTN) framework to determine the optimal operating conditions of multipurpose batch and continuous plants. Ierapetritou and Floudas (1998) introduced the original concept of unit specific events by introducing different task starting times in different units at the same event point. The formulation was defined as a basic two-index unit specific event based model considering unlimited intermediate storage policy where task spilling is not allowed. The formulation was based on the concept of decoupling the tasks from the unit events. Therefore, fewer numbers of event points are required as compared to the global event based models and slot based models. The minimum number of events leads to a smaller problem size that ultimately reduces the computational effort to a great extent. Majozi and Zhu (2001) presented a novel continuous-time MILP formulation based on state sequence network (SSN) representation for short term scheduling of batch plants with finite intermediate storage policies. In this SSN representation, by relating the input and output sates, the unit operations are included without using task notations. Maravelias and Grossmann (2003) generalized the global event based modelling approach for scheduling of batch plants by incorporating different batch process operational characteristics such as storage policies, batch splitting and mixing, utility resources and variable batch processing times. In the STN based model of Maravelias and Grossmann (2003) separate set of binary and continuous variables were defined for start, end, and continuation of tasks occurring over multiple events (a.k.a. task splitting). In the RTN based model of Castro et al., (2004) tasks were allowed to continue over multiple events using three-index sets of binary and continuous variables along with the option of controlling maximum number of global events over which a task is allowed to continue, thus, resulting in fewer number of global events compared to the model of Maravelias and Grossmann (2003). In both these models, a separate framework is not required for handling of resources due to global alignment of events. Sundaramoorthy and Karimi (2005) proposed a synchronized slot-based continuous time formulation for short-term scheduling of multipurpose batch plants with UIS and dedicated FIS storage policies. The mass balances were performed using slots as reference points to avoid the real time violations while using the limited shared resources. The proposed formulation does not require any Big-M constraints and eliminated the decoupling of tasks and units. Park and Kim (2004) proposed an MILP model for short term scheduling of non-sequential, single production line, multipurpose batch plants. The transfer and sequence dependent setup times were considered for the material states with four different storage policies. The task alignments were implemented using binary variables which were defined based on the production precedence between the products. Therefore, no additional binary variables were needed to handle the sequence dependent changeovers.

Floudas and co-authors (Janak et al., (2004); Janak et al., (2006); Shaik and Floudas(2007)) extended the unit specific event formulation proposed by Ierapetritou and Floudas (1998) for scheduling of batch and continuous processes considering various operational characteristics. Subsequently, Janak and Floudas (2008) proposed a unit-specific event based formulation with a set of preprocessing steps to reduce the integrality gap. It also allowed the reformulation linearization technique (RLT) to create sufficient and credible inequalities which can lead to tighter relaxation. Shaik and Floudas (2009) proposed a generic unified modelling approach for short term scheduling of batch plants with and without resources. The proposed model handles the task splitting using the three index binary and continuous variables. The parameter Δn value decides the task continuity over maximum number of events. In the absence of task splitting with the parameter Δn value equals to zero, the model reduces to simple case. Sundaramoorthy et al., (2009) proposed a discrete time MIP formulation for simultaneous batching and scheduling associated with different utility constraints such as limited availability of steam, cooling water and electricity. A common discrete time reference grid was adopted for accurate modeling of utility constraints. This technique also efficiently handles batching decisions (number and batch sizes), without the use of explicit variables for batch selection. Li et al., (2010) presented a detailed analysis of different unit specific event based models. The presented examples highlights the necessity of task splitting over multiple events to get the optimal solution. Pattinson and Majozi (2010) extended the SSN based continuous time model presented in Majozi and Zhu (2001) to synthesize, design and schedule of multipurpose batch plants. A new intermediate storage policy was introduced where the inactive process units at any time period were utilized for storing the intermediate material states. The proposed scheme enhanced the storage capacity for intermediate material states by effectively utilizing the dedicated storage and storage space in process units. The proposed Process Intermediate Storage (PIS) operational policy was effective in reducing the required dedicated FIS capacity for the specified throughput. Susarla et al., (2010) presented MILP model for short term scheduling of batch plants using unit-slots. This asynchronous slots behave similar to the unit specific events and handle different operational features with minimum number of slots. The proposed formulation has better computational efficiency compared to synchronous slot based model of Sundaramoorthy and Karimi (2005). Seid and Majozi (2012) proposed a unit specific time points based MILP model for short term scheduling of batch plants. SSN representation was used to define process flowsheet. For the first time, conditional sequencing concept was introduced where production and consumption tasks were aligned only when the material from production task is utilized by the consumption tasks. The proposed framework require less number of time points than the general unit specific event based models because of conditional alignment and unit wait policy. Kilic et al., (2011) proposed a discrete time MILP formulation for scheduling of multipurpose batch plants with shared storage capacity and storage time limitations. The discretization of time horizon, accurately monitored the lifespan of amount material in storage using simple model equations. However, because of inflexibility in timing decisions sub-optimal or even infeasible schedules may result.

The comparative studies presented in (Shaik and Floudas (2009); Li et al., (2010); Seid and Majozi (2012)) reveal that unit specific event based (multiple time grid) models are computationally superior to the global event and synchronous slot based models. Subsequently, Vooradi and Shaik (2012) improved the novel three index unit specific event based model proposed by Shaik and Floudas (2009) by incorporating the concept of active task. Using the active task concept, the allocation, duration and sequencing constraints were improved to enable the solution to large scale problems. Shaik and Vooradi (2013) proposed novel resource balance constraints that were offered unification across the STN and RTN based unit specific event based modelling frameworks for handling different resources such as material states, utilities, and equipment. The unification of resource handling resulted in further decrease in the number of events required. Vooradi and Shaik (2013) critically reviewed the concept of conditional sequencing proposed by Seid and Majozi (2012) and improvised the concept by enforcing the conditional sequencing only if the material or utility resource produced/released by production task is actually consumed/used by the consumption task. The proposed formulation resulted in better objective values and computational performance as compared to the unit specific event models with unconditional alignments. Lagzi et al., (2017) developed a slot based MILP formulation for scheduling of multipurpose plant operations. The proposed formulation considered the machines multitasking capabilities in process scheduling. Compared to single-tasking formulation, the multitasking formulations produce better optimal solution at the expense of more computational time. Lee and Maravelias (2017) proposed two discrete time mixed-integer programming models for batching and scheduling of multipurpose batch plants. The first modeling approach desegregate the orders into batches and each batch explicitly labeled and independently scheduled. In the second modeling approach, each batch was assigned to batch size intervals and an algorithm was proposed to identify the set of batch size intervals for every order. Shaik and Vooradi (2017) proposed a new configuration for unit specific event based modelling approach where the sequential production and consumption tasks were allowed to start at the same event, unlike in the conventional models where consumption task starts at the next event as compared to production task. The proposed concept further reduced the number of events required for scheduling of multipurpose batch plants without recycles. Mostafaei and Harjunkoski (2018) proposed a MILP formulation based on Generalized Disjunctive Programming (GDP) for multipurpose batch plants. Single-grid and multi-grid continuous models were derived using generalized disjunctive programming. As compared to the recent event based multiple time grid models, the proposed models using GDP resulted in a substantial reduction in solution time, problem size and tightening of linear relaxation. Rakovitis et al., (2019) extended the concept of production and consumption task at same event proposed in Shaik and Vooradi (2017) to solve twelve benchmark examples from the literature and compared the performance of the proposed model with Shaik and Floudas (2009).

2.2. Cyclic Scheduling of batch plants

Cyclic scheduling of multipurpose batch plants has significant attention in both industrial and academic domains, particularly while solving large scale problems. In cyclic scheduling, the longer time horizon is divided into cycles of equal time interval, thereby reducing the overall size of the problem. The splitting of the time horizon into smaller time intervals helps in focusing and producing the subset of products over a specific time period. This kind of approach helps in improving plant operation by the simultaneous implementation of necessary changes that are required to produce stable demand products. It also helps in establishing an operation schedule which can be executed repeatedly.

Different cyclic scheduling studies have been presented in the literature to derive the following important aspects: Shah et al., (1993) proposed a MILP mathematical model for cyclic scheduling of multi-purpose batch plants described by stream splitting & mixing, recycle, different storage policies and complex process networks. The STN based discrete time MILP formulation proposed by (Kondili et al., 1993) was extended to periodic scheduling of batch plants. The idea of task wrap-around accommodated the operational and modelling aspects of crossover tasks in a same cycle. Schilling and Pantelides (1999) proposed an RTN based MINLP model to find optimal cycle schedule for multipurpose plants consisting of batch, semi-batch, and continuous processes. The inherent approximations of discrete time models were eliminated by using a continuous-time framework and processing tasks were represented in more general form by considering batch dependent processing times. Castro et al., (2003) proposed discrete and continuous-time formulations for cyclic scheduling of pulp cooking industrial process and evaluated the performance of both models. It was observed that the discrete-time model was computationally superior to the continuous-time model for cyclic scheduling with constant batch processing times. Discrete time models sometime outperform continuous time models in terms of computational efficiency for the batch process with simple operational philosophies such as constant batch processing times, no stream splitting or mixing, dedicated resources etc. However, in general, continuous-time models are superior in handling complex batch operations such as variable batch processing times, variable fraction of production and consumption, presence of utility resources and different storage policies.

Wu and Ierapetritou (2004) proposed two index unit-specific event-based MINLP formulation to determine optimal cycle time and schedule for multipurpose batch plants. The proposed formulation extended the original unit specific event concept proposed by Ierapetritou and Floudas (1998) to cyclic scheduling of multipurpose batch plants. The formulation used two index binary and continuous variables to handle the material and energy balances. The formulation utilized the first event point to track the inventory of intermediates available at the cycle starting time. The formulation divided the entire time horizon into initial period, cyclic schedule and final period and each period was solved independently. Pochet and Warichet (2008) proposed a continuous-time global slot-based model for scheduling of large scale problems. The computational results emphasized that the MIP based relax-and-fix heuristic method was better than the truncated Branch and Bound method for solving large scale problems. Trautmann and Schwindt (2009) extended the cyclic scheduling concept to short term planning of batch plants. The proposed cyclic approach consists of three stages: cyclic batching, batch scheduling and concatenation. In cyclic batching the number of cycles and operational requirement in each cycle were identified. In cyclic scheduling priority rule based algorithm was used to schedule the batch process. In the third phase a complete production schedule is derived by connecting the batching and scheduling solutions. You et al., (2009) demonstrated the effectiveness of Dinkelbach's algorithm for cyclic scheduling of large scale problems. Various MINLP methods were also used to solve the Mixed Integer Linear Fractional Programming (MILFP) industrial problems. The computational performance of Dinkelbach's algorithm was found to be better than commercial MINLP solvers such as BARON, DICOPT, SBB and α-ECP.

He and Hui (2010) introduced a pattern matching method as an alternate to MILP and MINLP modelling approaches for solving large-scale multipurpose scheduling problems. A two stage decomposition approach was proposed which divides long time horizon into two sections. In the first section, pattern scheduling concept based on the principle of effective utilization of bottleneck units was used. In the second section, the remaining small duration was scheduled using MILP modelling techniques or heuristics. This decomposition approach did not increase the complexity of the problem and computational time with the problem size. Fumero et al., (2012) proposed a multiple time grid MILP slot based framework for scheduling of multistage batch plants operating under campaign mode. The proposed framework consists of two models. A simplified model was used to find the optimal cyclic time by considering preordering constraints. A rigorous scheduling model was used for finding the optimal schedule where the cycle time from the simplified model was used as an input parameter. This two stage framework reduced the computational burden significantly. Wu and Maravelias (2020) proposed a STN based MILP formulation for the periodic production scheduling. The effect of final product storage capacity on demand profiles and overall solution was systematically analyzed. The model can also handle the dynamic amount of utility availability and it's pricing.

2.3. Process scheduling and heat Integration

A large number of chemical industries fall in the realm of the highest energy-consuming industries. Hence, heat integration is essential for the efficient management of resources and minimization of waste (Stamp and Majozi(2011)). The striving efforts to reduce the energy utilization laid a strong foundation in the development of novel modeling techniques for batch process scheduling and heat integration. These batch process scheduling and heat integration modelling techniques can be classified into sequential and simultaneous frameworks. In a sequential framework the problem will be decomposed into two parts where the scheduling problem is solved first followed by heat integration problem. This decomposition reduces the problem complexity but it may leads to suboptimal solution. The simultaneous framework allows the interaction between scheduling and heat integration model equations and solves them simultaneously for global optimum (Halim and Srinivasan (2009)). Better optimum results may be obtained using simultaneous framework but they may have low computational efficiency due to large problem size. Both these configurations can handle direct and indirect heat integrations.

A number of modelling approaches have been proposed in literature to address various characteristics of scheduling and heat integration problem. Vaselenak et al., (1986) proposed a hybrid methodology for sequential process scheduling and heat integration of batch plants. A heuristic approach was presented to select a match between hot and cold tanks based on their initial temperatures. Further, in this approach, external utilities were used to heat or cool the tanks to their final desired temperatures. However, the proposed heuristic approach failed to provide an optimal solution, when the target temperatures are limiting. To handle this case efficiently, an MILP slot based formulation was proposed by considering final target temperatures. Ivanov et al., (1992) and Peneva et al., (1992) proposed non-linear formulations for heat integration of batch plant to maximize the energy exchange potential by combining the direct heat integration with temperature corrections by using external agents. The proposed formulations can be integrated with batch plant design or retrofitting to ensure maximum energy utilization. Corominas et al., (1993) proposed a sequential framework by introducing a concept of macro network for the heat integration of batch processes operating in different campaigns. The campaigns containing different batches are examined to find the best hot and cold stream match to achieve maximum heat exchange. Papageourgiou et al., (1994) first proposed an MINLP discrete time model for simultaneous scheduling and heat integration of batch as well as semi continuous plants. The direct and indirect heat integration characteristics were separately incorporated with the general scheduling framework proposed by (Kondili et al., 1993). A branch and bound solution approach was used to solve the resulting non-convex MINLP problem. Lee and Reklaitis (1995) proposed MILP formulation for simultaneous scheduling and heat integration of single product batch process with finite wait storage policy. The heat exchange pairing between the hot and cold streams was limited to one to one matching. Zhao et al., (1998) proposed MINLP model for simultaneous scheduling and heat integration of batch processes operated cyclically. Heat exchange potential was increased by allowing energy transfer from one to multiple streams. Vaklieva-Bancheva et al., (1996) proposed a sequential framework for designing the optimal cost heat exchange networks for multistage batch plants taking into account both operating and capital costs. Direct heat integration and product campaign selections were simultaneously modelled as MILP problems to ensure a global optimal solution. Barbosa-Povoa et al., (2001) extended the design model presented in Barbosa-Povoa and Macchietto (1994) by introducing the direct heat integration concept at batch plant design stage to facilitate the close interaction between different operational aspects, heat integration policies and associated auxiliary units. Pinto and Novais (2003) extended the design and heat integration modelling approach proposed by (Barbosa-Povoa et al., 2001) by considering economic savings associated with different utility components such as auxiliary structures, utility circuits and associated piping costs. A State Task Network (STN) based discrete time MILP model was proposed, in which binary variables define operational & topological decisions and continuous variables define the task durations, material and energy balances. Adonyi et al., (2003) proposed an S-graph approach for scheduling and heat integration of batch plants with no intermediate storage policy. Using branch and bound algorithms the scheduling and heat integration problems were simultaneously solved.

Majozi (2006) proposed a continuous time MILP formulation using State Sequence Network (SSN) framework for simultaneous scheduling and direct heat integration of batch plants. Single time grid modeling approach was used in the proposed formulation. This formulation is applicable to multipurpose and multiproduct batch facilities. The batch processes with constant and variable amount of energy requirements were handled using the bilinear energy balance equations. In the second case the energy requirement vary linearly with batch size. The formulation resulted in better model statistics and computational performance compared to the discrete time formulation presented by (Papageorgiou et al., 1994). In the year 2009, Majozi extended his formulation by incorporating indirect heat integration, where thermal fluid was used to exchange heat with process streams at different time intervals (Majozi, 2009). Significant reduction in external utilities (hot and cold) was observed for the plants with indirect heat integration which allows the energy exchange between active non coexisting heating and cooling tasks. Chen and Chang (2009) proposed a RTN based continuous time formulation for simultaneous short-term/periodic scheduling and heat integration of multipurpose batch plants. The direct heat integration concepts from Majozi (2006) and short term scheduling concepts from Castro et al., (2003) and (2004) were used to develop unified global event based model. Halim and Srinivasan (2009) proposed a three stage sequential methodology for batch process scheduling and heat integration problem. At the first stage scheduling problem was solved for the objective such as makespan or profit. Next, using a stochastic search based integer cut procedure a set of near optimal schedules were generated. Finally, heat integration analysis was carried to find the minimum utility target for each of the resulting schedule. This three stage procedure relaxed the concept of retaining scheduling problem optimal solution while solving the heat integration problem.

Stamp and Majozi (2011) extended the Majozi (2009) model by optimizing the amount of thermal fluid and initial temperature. Trilinear terms were used to calculate enthalpy change of the thermal fluid during heat exchange. Significant external utility savings were observed with optimal amount of thermal fluid and initial temperature. However, the initial condition of heat storage vessel and associated cost were not included in the optimization. Seid and Mazoji (2014) improved the heat integration model of Majozi (2006) based on robust scheduling framework of Seid and Majozi (2012). By incorporating a heat storage vessel, the model proved that there is a significant reduction in utility consumption. The improved scheduling model is based on State Sequence Network (SSN), handled indirect heat integration effectively by adding new constraints. Castro et al., (2015) proposed a continuous-time MILP model based on general precedence variables for addressing scheduling and heat integration of single-stage plants. A clear trade-off was observed between the two objectives of minimization of makespan and external utility savings. Lee et al., (2016) proposed an MINLP unit specific event based model for simultaneous scheduling and heat integration of multipurpose batch plants by facilitating the heat exchange during the material transfer between the processing units. This formulation allows heat integration between the intermediate material states before or after storage. These operational flexibilities resulted in higher production rates and lower external utilities. Stamp and Majozi (2017) proposed MINLP model for cyclic scheduling and heat integration of batch plants. The SSN framework was developed by combining the heat integration concepts presented by Stamp and Majozi (2011) and cyclic scheduling concepts proposed by Wu and Ierapetritou (2004). A single heat storage vessel was considered for exchanging heat with process streams. Sebelebele and Majozi (2017) proposed a unit specific event based model for heat integration of batch plants using multiple storage vessels. The main emphasis is on feasibility of indirect heat integration during the optimal heat storage vessels design. However, the formulation failed in highlighting the advantage of simultaneous direct and indirect heat integration. Magege and Majozi (2020) proposed a MINLP model for batch plant design, scheduling and intermittent stream heat integration. The movement of intermittently available streams were precisely monitored using the STN framework. The proposed formulation explored the heat exchange possibilities using superstructure at the design stage.

2.4. Research gaps

From the presented literature, it is evident that new modeling techniques for simultaneous scheduling and heat integration of batch processes have been proposed to improve the model performance. Few robust scheduling models from the literature are also extended to handle simultaneous heat integration. Based on the above literature review the following research gaps are identified.

- From the above literature it is observed that for obtaining optimal solution to a given scheduling problem, in general USEB models require less number of events, variables and constraints as compared to global-event and slot-based models. Hence they have computationally better performance than the other modeling approaches. However, the USEB models have complex structure to handle the heterogeneity of events across units. Therefore, still there is further scope to improve the USEB model structure and the computational performance. Further, these models are not well explored for addressing the issues associated with cyclic scheduling and heat integration.
- Extensive studies were available in the literature for the handling of batch process scheduling with heat integration. Limited studies (Chen and Chang (2009); Stamp and Majozi (2017)) have embedded the concept of heat integration with cyclic scheduling using single time grid modeling approach to reduce the complexity while solving large scale problems. Multiple time grid modelling approaches are not well explored to handle simultaneous cyclic scheduling and heat integration of batch plants.
- Rigorous multiple time grid modelling approaches have been proposed in literature to address different operational characteristics of batch process scheduling. Simultaneous scheduling and heat integration has a significant scope for further study by including a wide variety of commonly encountered heat integration features such as heat losses, simultaneous heating and cooling, property changes with temperature and heat transfer rates. Moreover, most of the simultaneous scheduling and heat integration problems were solved using single time grid modelling approach. Only a handful of research works highlighted the computational effectiveness of multiple time grid modelling approach for simultaneous scheduling and heat integration of batch plants (Lee et al., (2015), (2016)); Seid and Majozi (2014); Stamp and Majozi (2017)). Better optimal results may be obtained by i) effectively handling different heat integration features such as possible combination of direct and indirect heat integration ii) design and optimization of heat storage vessels and iii) improving the computational performance of the model.

2.5. Research objectives

The following research objectives are formulated to meet the above mentioned research gaps.

2.5.1. Objective 1: To propose three index USEB model for short term scheduling of batch plants with direct heat integration

The objective is to extend the USEB model proposed by Vooradi and Shaik (2012) to handle simultaneous batch process scheduling and direct heat integration. The major emphasis is on the inclusion of novel model equations using active task concept to improve model statistics and computational performance compared to the existing models available in the literature.

2.5.2. Objective 2: To propose unified USEB model for cyclic scheduling and heat integration of batch plants

The objective is to propose a novel three index unified USEB model to handle the short term and cyclic scheduling of batch processes. The unified model must reduce to simple scheduling framework in the absence of cyclic scheduling by restricting task continuity to the next cycle. The proposed cyclic scheduling model will be extended to handle simultaneous direct heat integration.

2.5.3. Objective 3: To propose a simple USEB framework for short term scheduling and heat integration batch plants with design and optimization of heat storage vessels

The main objective of this work is to optimize the use of direct and indirect heat integration in batch plants, as this is a scenario more often encountered in industrial applications. To meet this objective, a unit specific event based (multiple time grid) framework is to be proposed for simultaneous scheduling and heat integration of batch plants considering design and optimization of heat storage vessels.

2.5.4. Objective 4: To propose a USEB model for simultaneous cyclic scheduling and heat integration of batch plants considering design and optimization of heat storage vessels

The main objective is to optimize the use of direct and indirect heat integration in batch plants having long term scheduling horizons, as this is commonly encountered in industrial applications. Towards this end, a unit specific event based framework is to be proposed for simultaneous cyclic scheduling and heat integration of batch plants with design and optimization of heat storage vessels. The final goal, as in case of all the other optimization problems, is to improve the net profit, considering the important industrial constraints.

This chapter presented up to date modelling developments on the short-term scheduling of batch plants with different storage policies and utility resources, cyclic scheduling of batch plants, and process scheduling & heat integration. At the end, the identified research gaps along with the proposed four objectives to address these gaps are presented. Chapters 3, 4, 5 and 6 are designed as working chapters, where theoretical developments are presented to fulfill the objectives one to four respectively. In these chapters the performance of the proposed formulations is compared with literature models by solving benchmark examples.

CHAPTER 3

SIMULTANEOUS SCHEDULING AND DIRECT HEAT INTEGRATION OF BATCH PLANTS USING UNIT SPECIFIC EVENT BASED MODELLING

Simultaneous scheduling and direct heat Integration of batch plants using unit specific event based modelling

In recent days the swift increase of chemical industrialization is associated with sustainability measures in profit, product purity and environmental concerns. In general, the batch processes are considered to be important with amenable productivity due to their inherent operational advantages: less complexity, flexibility in operation, efficient usage of energy and easy in control. Thus, batch plants still have an edge over continuous plants for small scale production. In addition to it batch plants can produce multiple products by effectively utilizing the available common resources. Therefore, process scheduling and heat integration plays a predominant role in most of the chemical industries to address the factors such as energy efficiency, profit maximization and cost minimization by minimizing the unit idle times and energy losses.

From the presented literature in chapter two, it is evident that new modeling techniques for batch process scheduling and heat integration have been proposed to improve the model performance. The robust scheduling models such as (Majozi and Zhu (2001); Seid and Majozi (2012)) are extended to handle simultaneous scheduling and heat integration. Unit specific event based (USEB) modeling approach proposed by Ierapetritou and Floudas (1998) has become one of the popular framework to handle the different scheduling aspects (Janak and Floudas(2008); Li and Floudas(2010); Shaik and Floudas(2009); Vooradi and Shaik (2012)). This approach require minimum number of event points to get the optimal schedule as compare to global event based models and slot based models. Rigorous USEB mathematical models have been proposed in the literature for short term scheduling of batch plants and computational performance of these models are compared with slot and global event formulations. Subsequently, the USEB modeling approach has not been extended to handle the simultaneous scheduling and heat integration of batch plants. Hence, in this chapter a three index USEB model is proposed to handle simultaneous process scheduling and direct heat integration of batch processes. The major emphasis is on the inclusion of novel model equations to improve model statistics and computational performance compared to the existing models available in the literature. The computational performance of the proposed formulation is compared with the Chen and Chang (2009) model through various examples drawn from the literature. The rest of the chapter is organized as follows. In section 3.1, the problem statement for simultaneous scheduling and direct heat integration is presented. In section 3.2, three index USEB model is proposed and in sections 3.3 two examples are solved to demonstrate the effectiveness of the proposed approach.

3.1. Problem statement

The brief description of the scheduling problem that has been addressed in this chapter is as follows. Given: (i) process and production data, including size and magnitude of equipment, material flows, etc., duration of the task, product recipes, time horizon, raw materials cost, selling price of final products and cost incurred on operations (operating cost) (ii) task specific amount of hot and cold utility requirements and (iii) cost incurred for cold and hot utilities. The objective is to determine (i) A heat integrated production schedule with maximum profit or minimum makespan (ii) Minimum external utility requirements (iii) The material processed by different tasks in different units and (iv) The task start and finish times. The following assumptions are considered: zero material transfer time, no unit failures, heat exchanger capital cost is not considered in profit maximization and pre-processing material waiting is not allowed.

3.2. Mathematical formulation

The methodology presented in this chapter is based on unit specific event based continuous-time model proposed by Vooradi and Shaik (2012). The proposed model is applicable to both multiproduct and multipurpose batch processes and it can handle the standalone and/or heat integration aspects with variable batch sizes. The presented mathematical formulation uses state task network (STN) representation and consists of the following scheduling and heat integration equations.

3.2.1. Allocation Constraints

$$\sum_{i \in I_j} \sum_{\substack{n2 \in N \\ n1-\Delta n \leq n2 \leq n1}} \sum_{\substack{n3 \in N \\ n2 \leq n3 \leq n2+\Delta n}} w(i,n2,n3) \leq 1, \quad \forall\ j \in J, n1 \in N \tag{3.1}$$

The constraint (3.1) describes the occurrence of task *i* in unit *j* and ensures that at the maximum one task can only be active in each unit at the event point *n*.

3.2.2. Batch Size Constraints

$$B_i^{min} w(i,n1,n2) \leq b(i,n1,n2) \leq B_i^{max} w(i,n1,n2),$$
$$\forall\ i \in I, n1, n2 \in N, B_i^{min}, n1 \leq n2 \leq n1 + \Delta n \tag{3.2}$$

The amount of material processed by task *i* in unit *j* should be within the limits of minimum and maximum batch size as shown in equation (3.2).

3.2.3. Material Balances

Constraint (3.3) calculates the material state *s* available in storage at event *n* which is equal to sum of the amount available in storage at event *n*-1 and amount produced at event point *n*-1 minus amount consumed at event *n*. The equation (3.4) can be used for the material balance at first event.

$$ST(s,n1) = ST(s,n1-1) + \sum_{i \in I_s^p} \rho_{is} \sum_{\substack{n2 \in N \\ n1-1-\Delta n \le n2 \le n1-1}} b(i,n2,n1-1) +$$

$$\sum_{i \in I_s^c} \rho_{is} \sum_{\substack{n2 \in N \\ n1 \le n2 \le n1+\Delta n}} b(i,n1,n2), \quad \forall \ s \in S, n1 \in N, n1 > 1 \qquad (3.3)$$

$$ST(s,n1) = ST_0(s) + \sum_{i \in I_s^c} \rho_{is} \sum_{\substack{n2 \in N \\ n1 \le n2 \le n1+\Delta n}} b(i,n1,n2), \quad \forall \ s \in S, n1 \in N, n1 = 1 \qquad (3.4)$$

3.2.4. Task Duration Constraints

At Δn=0, the task finish time of task *i* at event *n1* is calculated using constraint (3.5).

$$T^f(i,n1) = T^s(i,n1) + \gamma_i w(i,n1,n1) + \delta_i b(i,n1,n1),$$

$$\forall \ i \in I, n1 \in N, \Delta n = 0 \qquad (3.5)$$

The constraints (3.6) and (3.7) are used to calculate the finishing time of task *i* that is active over multiple events.

$$T^f(i,n2) \ge T^s(i,n1) + \gamma_i w(i,n1,n2) + \delta_i b(i,n1,n2),$$

$$\forall \ i \in I, n1, n2 \in N, n1 \le n2 \le n1 + \Delta n, \Delta n > 0 \qquad (3.6)$$

$$T^f(i,n2) \le T^s(i,n1) + \gamma_i w(i,n1,n2) + \delta_i b(i,n1,n2) + M\big(1 - w(i,n1,n2)\big),$$

$$\forall \ i \in I, n1, n2 \in N, n1 \le n2 \le n1 + \Delta n, \Delta n > 0 \qquad (3.7)$$

3.2.5. Alignment Constraints

Equation (3.8) aligns the starting time of task *i* at event *n1*+1 with the finish time of the same task at event *n1*.

$$T^s(i,n1+1) \ge T^f(i,n1), \qquad \forall \ i \in I, n1 \in N, n1 < N \qquad (3.8)$$

Constraint (3.9) aligns the finishing time of task *i* at event *n1* with the start time at event *n1*+1 if the task is active at these two events.

$$T^s(i,n1+1) \le T^f(i,n1) + M\left(1 - \sum_{\substack{n2 \in N \\ n1-\Delta n \le n2 \le n1}} \sum_{\substack{n3 \in N \\ n2 \le n3 \le n2+\Delta n}} w(i,n2,n3)\right),$$

$$\forall \ i \in I, n1 \in N, n1 < N, \Delta n > 0 \qquad (3.9)$$

The constraint (3.10) relates the start of task *i* at event *n1*+1 and finish time of task *i1* at event *n1* in the unit *j*.

$$T^s(i,n1+1) \ge T^f(i1,n1), \qquad \forall \ i, i1 \in I_j, i \ne i1, j \in J, n1 \in N, n1 < N \qquad (3.10)$$

The constraint (3.11) is used to align different tasks *i* and *i*1 performing in different units *j* and *j*1. It states that starting time of consumption task at event *n*1+1 must be greater than the finishing time of a production the task at event *n*1.

$$T^s(i,n1+1) \ge T^f(i1,n1) - M\left(1 - \sum_{\substack{n2 \in N \\ n1-\Delta n \le n2 \le n1}} w(i1,n2,n1)\right), \qquad \forall \ s \in S, i \in I_j,$$

$$i1 \in I_{j1}, i \in I_s^c, i1 \in I_s^p, i \ne i1, j, j1 \in J, j \ne j1, n1 \in N, n1 > \Delta n, n1 < N \qquad (3.11)$$

3.2.6. Different storage policies

The following constraint (3.12) presents no-wait condition needed for finite intermediate storage state by aligning the production and consumption tasks.

$$T^s(i, n1+1) \leq T^f(i1, n1) + M\left(2 - \sum_{\substack{n2 \in N \\ n1-\Delta n \leq n2 \leq n1}} w(i1, n2, n1) - \sum_{\substack{n2 \in N \\ n1+1 \leq n2 \leq n1+1+\Delta n}} w(i, n1+1, n2)\right),$$

$$\forall \ s \in S^{fis}, i \in I_j, i1 \in I_{j1}, i \in I_s^c, i1 \in I_s^p, i \neq i1, j, j1 \in J, j \neq j1, n1 \in N, n1 < N \quad (3.12)$$

Constraint (3.13) eliminates the real time storage violation for finite intermediate storage states.

$$T^f(i1, n1) \geq T^s(i, n1) - M\left(2 - \sum_{\substack{n2 \in N \\ n1-\Delta n \leq n2 \leq n1}} w(i1, n2, n1) - \sum_{\substack{n2 \in N \\ n1-\Delta n \leq n2 \leq n1}} \sum_{\substack{n3 \in N \\ n2 \leq n3 \leq n2+\Delta n}} w(i, n2, n3)\right),$$

$$\forall \ s \in S^{fis}, i \in I_j, i1 \in I_{j1}, i \in I_s^c, i1 \in I_s^p, i \neq i1, j, j1 \in J, j \neq j1, n1 \in N, n1 < N \quad (3.13)$$

3.2.7. Heat integration constraints

Constraint (3.14) and (3.15) ensures heat integration between the tasks that require cooling and heating. The binary variable $x(i, i1, n1)$ value of one indicates that there is energy transfer from task *i1* to task *i*.

$$\sum_{i1 \in I_c} x(i, i1, n1) \leq \sum_{\substack{n2 \in N \\ n1 \leq n2 \leq n1+\Delta n}} w(i, n1, n2), \quad \forall \ i \in I_h, i \neq i1, n1 \in N \quad (3.14)$$

$$\sum_{i \in I_h} x(i, i1, n) \leq \sum_{\substack{n2 \in N \\ n1 \leq n2 \leq n1+\Delta n}} w(i1, n1, n2), \quad \forall \ i1 \in I_c, i \neq i1, n1 \in N \quad (3.15)$$

Constraints (3.16) and (3.17) calculate the amount of hot utility required for task *i*. Constraint (3.16) describes the energy balance for standalone task, whereas constraint (3.17) represents the energy balance for the heat integrated task. Similarly constraints (3.18) and (3.19) calculate the amount of cold utility required for standalone and heat integrated tasks respectively.

$$q(i, n1) = \alpha_i\left(\sum_{\substack{n2 \in N \\ n1 \leq n2 \leq n1+\Delta n}} w(i, n1, n2) - \sum_{i1 \in I_c} x(i, i1, n1)\right) + \beta_i \sum_{\substack{n2 \in N \\ n1 \leq n2 \leq n1+\Delta n}} b(i, n1, n2)$$

$$\left(\sum_{\substack{n2\in N\\ n1\le n2\le n1+\Delta n}} w(i,n1,n2) - \sum_{i1\in I_c} x(i,i1,n1)\right), \qquad \forall \;\; i\in I_h, i\ne i1, n1\in N \qquad (3.16)$$

$$q1(i,n1) = \alpha_i' \sum_{i1\in I_c} x(i,i1,n1) + \beta_i' \sum_{\substack{n2\in N\\ n1\le n2\le n1+\Delta n}} b(i,n1,n2) \sum_{i1\in I_c} x(i,i1,n1),$$

$$\forall \;\; i\in I_h, i\ne i1, n1\in N \qquad (3.17)$$

$$q(i1,n1) = \alpha_{i1}\left(\sum_{\substack{n2\in N\\ n1\le n2\le n1+\Delta n}} w(i1,n1,n2) - \sum_{i\in I_h} x(i,i1,n1)\right) + \beta_{i1}$$

$$\sum_{\substack{n2\in N\\ n1\le n2\le n1+\Delta n}} b(i1,n1,n2) + \left(\sum_{\substack{n2\in N\\ n1\le n2\le n1+\Delta n}} w(i1,n1,n2) - \sum_{i\in I_h} x(i,i1,n1)\right),$$

$$\forall \;\; i1\in I_c, i\ne i1, n1\in N \qquad (3.18)$$

$$q1(i1,n1) = \alpha_{i1}' \sum_{i\in I_h} x(i,i1,n) + \beta_{i1}' \sum_{\substack{n2\in N\\ n1\le n2\le n1+\Delta n}} b(i1,n1,n2) \sum_{i\in I_h} x(i,i1,n1),$$

$$\forall \;\; i1\in I_c, i\ne i1, n1\in N \qquad (3.19)$$

The constraints (3.16) to (3.19) involve bilinear terms containing both binary and continuous variables. These terms can be linearized using Glover transformation and linear optimization can be applied to obtain overall optimal schedule. The bilinear terms in the constraints (3.16) to (3.19) are replaced by only two variables $bh(i,i1,n1)$ and $bc(i,i1,n1)$. The energy balance equations are rewritten using these linear variables as shown in the constraints (3.20) to (3.23).

$$q(i,n) = \alpha_i\left(\sum_{\substack{n2\in N\\ n1\le n2\le n1+\Delta n}} w(i,n1,n2) - \sum_{i1\in I_c} x(i,i1,n1)\right) +$$

$$\beta_i\left(\sum_{\substack{n2\in N\\ n1\le n2\le n1+\Delta n}} b(i,n1,n2) - \sum_{i1\in I_c} bh(i,i1,n1)\right), \qquad \forall \;\; i\in I_h, i\ne i1, n1\in N \qquad (3.20)$$

$$q(i1,n) = \alpha_{i1}\left(\sum_{\substack{n2\in N\\ n1\le n2\le n1+\Delta n}} w(i1,n1,n2) - \sum_{i\in I_h} x(i,i1,n1)\right) +$$

$$\beta_{i1}\left(\sum_{\substack{n2\in N\\ n1\le n2\le n1+\Delta n}} b(i1,n1,n2) - \sum_{i\in I_h} bc(i,i1,n1)\right), \qquad \forall \;\; i1\in I_c, i\ne i1, n1\in N \qquad (3.21)$$

$$q1(i,n1) = \alpha_i' \sum_{i1 \in I_c} x(i,i1,n1) + \beta_i' \sum_{i1 \in I_c} bh(i,i1,n1)\ , \quad \forall \ \ i \in I_h, i \neq i1, n1 \in N \qquad (3.22)$$

$$q1(i1,n1) = \alpha_{i1}' \sum_{i \in I_h} x(i,i1,n1) + \beta_{i1}' \sum_{i \in I_h} bc(i,i1,n1)\ , \forall \ \ i1 \in I_c, i \neq i1, n1 \in N \qquad (3.23)$$

The constraints (3.24) to (3.27) define the bilinear variables *bh*(*i*,*i1*,*n1*) and *bc*(*i*,*i1*,*n1*) using suitable batch processing amounts when the tasks *i* and *i1* are integrated. In the absence of integration, zero is assigned to these variables.

$$B_i^{min} x(i,i1,n1) \leq bh(i,i1,n1) \leq B_i^{max} x(i,i1,n1), \qquad \forall \ \ i \in I_h, i1 \in I_c, n1 \in N \qquad (3.24)$$

$$\sum_{\substack{n2 \in N \\ n1 \leq n2 \leq n1+\Delta n}} b(i,n1,n2) - \ B_i^{max}\big(1 - x(i,i1,n1)\big) \leq bh(i,i1,n1)$$
$$\leq \sum_{\substack{n2 \in N \\ n1 \leq n2 \leq n1+\Delta n}} b(i,n1,n2), \qquad \forall \ \ i \in I_h, i1 \in I_c, n1 \in N \qquad (3.25)$$

$$B_{i1}^{min} x(i,i1,n1) \leq bc(i,i1,n1) \leq B_{i1}^{max} x(i,i1,n1), \qquad \forall \ \ i \in I_h, i1 \in I_c, n1 \in N \qquad (3.26)$$

$$\sum_{\substack{n2 \in N \\ n1 \leq n2 \leq n1+\Delta n}} b(i1,n1,n2) - \ B_{i1}^{max}\big(1 - x(i,i1,n1)\big) \leq bc(i,i1,n1)$$
$$\leq \sum_{\substack{n2 \in N \\ n1 \leq n2 \leq n1+\Delta n}} b(i1,n1,n2), \qquad \forall \ \ i \in I_h, i1 \in I_c, n1 \in N \qquad (3.27)$$

Constraints (3.28) and (3.29) state that the starting time of task *i* which requires heating should happen one hour after the starting time of task *i1* which requires cooling when they are in heat integration mode.

$$T^s(i,n1) \geq 1 + T^s(i1,n1) - M\big(1 - x(i,i1,n1)\big), \qquad \forall \ \ i \in I_h, i1 \in I_c, n1 \in N \qquad (3.28)$$

$$T^s(i,n1) \leq 1 + T^s(i1,n1) + M\big(1 - x(i,i1,n1)\big), \qquad \forall \ \ i \in I_h, i1 \in I_c, n1 \in N \qquad (3.29)$$

When the task duration changes with heat integration, the constraints (3.30) and (3.31) are used to calculate the finishing times of heat integrated tasks. If $\Delta n>0$, then the constraints (3.32) to (3.35) are used to align the heat integrated tasks.

$$T^f(i,n1) = T^s(i,n1) + \gamma_i \left(w(i,n1,n1) - \sum_{i1 \in I_c} x(i,i1,n1) \right) + \gamma_i' \sum_{i1 \in I_c} x(i,i1,n1)\ ,$$
$$\forall \ \ i \in I_h, i \neq i1, n1 \in N, \Delta n = 0 \qquad (3.30)$$

$$T^f(i1,n1) = T^s(i1,n1) + \gamma_{i1} \left(w(i1,n1,n1) - \sum_{i \in I_h} x(i,i1,n1) \right) + \gamma_{i1}' \sum_{i \in I_h} x(i,i1,n1)\ ,$$
$$\forall \ \ i1 \in I_c, i \neq i1, n1 \in N, \Delta n = 0 \qquad (3.31)$$

$$T^f(i,n2) \geq T^s(i,n1) + \gamma_i \left(w(i,n1,n2) - \sum_{i1 \in I_c} x(i,i1,n1) \right) + \gamma_i' \sum_{i1 \in I_c} x(i,i1,n1)$$

$$-M\big(1 - w(i,n1,n2)\big), \quad \forall \;\; i \in I_h, i \neq i1, n1, n2 \in N, n1 \leq n2 \leq n1 + \Delta n, \Delta n > 0 \qquad (3.32)$$

$$T^f(i,n2) \leq T^s(i,n1) + \gamma_i \left(w(i,n1,n2) - \sum_{i1 \in I_c} x(i,i1,n1) \right) + \gamma_i' \sum_{i1 \in I_c} x(i,i1,n1)$$

$$+M\big(1 - w(i,n1,n2)\big), \quad \forall \;\; i \in I_h, i \neq i1, n1, n2 \in N, n1 \leq n2 \leq n1 + \Delta n, \Delta n > 0 \qquad (3.33)$$

$$T^f(i1,n2) \geq T^s(i1,n1) + \gamma_{i1} \left(w(i1,n1,n2) - \sum_{i \in I_h} x(i,i1,n1) \right) + \gamma_{i1}' \sum_{i \in I_h} x(i,i1,n1)$$

$$-M\big(1 - w(i1,n1,n2)\big), \;\; \forall \;\; i1 \in I_c, i \neq i1, n1, n2 \in N, n1 \leq n2 \leq n1 + \Delta n, \Delta n > 0 \qquad (3.34)$$

$$T^f(i1,n2) \leq T^s(i1,n1) + \gamma_{i1} \left(w(i1,n1,n2) - \sum_{i \in I_h} x(i,i1,n1) \right) + \gamma_{i1}' \sum_{i \in I_h} x(i,i1,n1)$$

$$+M\big(1 - w(i1,n1,n2)\big), \;\; \forall \;\; i1 \in I_c, i \neq i1, n1, n2 \in N, n1 \leq n2 \leq n1 + \Delta n, \Delta n > 0 \qquad (3.35)$$

3.2.8. Objective Function:

The objective function shown in equation (3.36) is the maximization of profit which is the difference between revenue from the products and operating cost. The operating cost involves the expenses incurred on use of external utilities including steam and cooling water. This profit maximization is sensitive to the amount of final product produced and amount of utilities required. These two variables influence the occurrence of processing tasks and heat integration between them.

$$Maxprofit \;\; Z = \sum_{s \in S^p} price(s) \left(\sum_{n1=N} ST(S,n1) + \sum_{i \in I_s^p} \rho_{is} \sum_{\substack{n2 \in N \\ n1-\Delta n \leq n2 \leq n1}} b(i,n2,n1) \right)$$

$$-\sum_{i \in I_h} \sum_{n1=1}^{N} \big(c_{uh} q(i,n1)\big) - \sum_{i \in I_c} \sum_{n1=1}^{N} \big(c_{uc} q(i,n1)\big), \qquad (3.36)$$

3.2.9. Important enhancements of the proposed formulations

- Three index unit specific event formulation for batch process scheduling proposed by Vooradi and Shaik (2012) is extended to handle simultaneous scheduling and direct heat integration of batch plants.
- In utility balance equations, the linearization of bilinear terms is handled by using Glover transformation with minimum number of variables and constraints.

- The heterogeneous location of event points on time horizon and task splitting allow the formulation with independent heat integration constraints to handle simultaneous scheduling and direct heat integration.

3.3. Computational case study

The feasibility of the proposed model is demonstrated by solving two benchmark examples. The model statistics and computational results of the standalone and heat integrated case studies have been compared with the Chen and Chang (2009) model. However, in this work, the CPU time of Chen and Chang (2009) model is reported for completeness only and not for direct comparison because the computational resources used in the present work are different. The model is executed using GAMS 24.4.1/CPLEX solver in desktop computer with Intel Xeon E5-1607 3.00 Ghz processor and 8 GB RAM. To obtain the optimal solution, the model is iteratively solved over different numbers of events.

3.3.1. Example 3.1

The benchmark example discussed in Chen and Chang (2009) is considered in this work. Fig. 3.1 describes the production process using STN representation. The feed mixture comprising of 60% Feed 1 (S1) and 40% Feed 2 (S2) is fed to a reactor for carrying out the reaction. The reaction is exothermic hence heat is liberated during the reaction. Cold water is used as a cooling medium to control the reactor temperature. The intermediate (S3) produced in the rector is fed to the filtration unit to separate unwanted waste. The filtered product (S4) is fed to the distillation column and a product consisting of 75% product A and 25% product B is obtained. Steam is used as a hot utility in reboiler unit attached to the distillation column. The problem data including unit capacity, utility requirement, task duration, and task-unit assignment is given in Table 3.1. The minimum size of the batch amount processed in reactor and distillation units cannot be less than 25% of its capacity. Whereas for filtration unit it should not be less than 10% of its capacity.

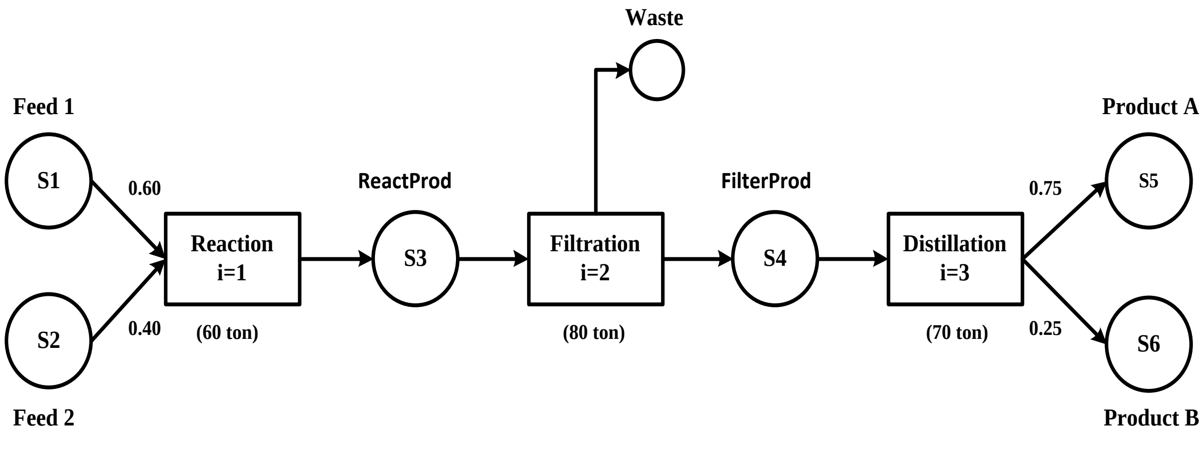


Fig. 3.1. STN for Example 3.1

Table 3.1. Data for Example 3.1

Unit (j)	Task (i)	Processing Time(h)	Capacity (tons)	Operation Mode	Utilities Requirement	Amount (tons/h)
Reactor (j1)	Reaction	2	60	Without Heat Integration	Cold water	1.59+0.1Bt/h
		3		With Heat Integration	Cold water	1.0+0.06 Bt/h
Filter (j2)	Filtration	1	80	Without Heat Integration	None	0 t/h
Distiller (j3)	Distillation	2	70	Without Heat Integration	Steam	0.044+0.0035Bt /h
		2		With Heat Integration	Steam	0.020+0.0016 B t/h

The minimum size of the batch amount processed in reactor and distillation units cannot be less than 25% of its capacity. Whereas for filtration unit it should not be less than 10% of its capacity. The two intermediate material states S3 and S4 are having a finite storage capacity of 100 tons for each state. The storage capacity of raw materials and final products is assumed to be unlimited. It is also assumed that sufficient amount of hot and cold utilities are available. The operational cost associated with the utilities steam and cold water is 200 and 4 relative cost units per ton (rcu / ton) respectively. The products selling price is 5 rcu / ton. The example is solved with the objective of profit maximization considering 48 hours of time horizon. The computational results for both standalone and heat integrated case studies are presented in Table 3.2.

Table 3.2. Computational results for Example 3.1

	Standalone		**Heat integration**	
Model used	Chen and Chang (2009)	The Proposed USEB model	Chen and Chang (2009)	The Proposed USEB model
Time points/Events	25	24	32	27
Objective value	3081.8	3081.8	3644.6	3644.6
RMILP	--[a]	3084.2	--[a]	3857.2
CPU time(sec)	0.375[b]	0.203	272[b]	35.63
Product1(tons)	990	990	720	720
Product2(tons)	330	330	240	240
Steam(tons)	10.9	10.9	3.6	3.6
Cooling water(tons)	334	334	107.2	107.2
Binary variables	72	72	244	104
Continuous variables	--[a]	367	--[a]	566
Constraints	--[a]	640	--[a]	1141

[a]Not reported, [b]CPU time for Chen and Chang (2009) model is given for completeness only

3.3.1.1. Standalone mode

In standalone mode, the required utility load for distillation and reactor tasks is supplied by using external resources steam and cold water. The proposed model requires 24 events to obtain an objective value of 3081.8. A total product of 1320 tons is produced, out of which 990 tons of product-1 and 330 tons of product-2 are obtained. The cost involved in this operation for utilities including steam for heating and cold water for cooling are 2180 and

1330 rcu respectively. The optimal Gantt chart for the case of without heat integration is shown in Fig. 3.2. In the Gantt chart, the x-axis represent real time horizon in hours and y-axis represent processing units. The processing tasks are highlighted by using three identifiers including task number at the bottom, batch processing amount at the top and event number on the left side. The Gantt chart can be read with the help of these three identifiers. For instance, in Fig. 3.2 at event *n1* the task one is active in unit *j1* and it is processing 60 tons of material in 2 hours duration.

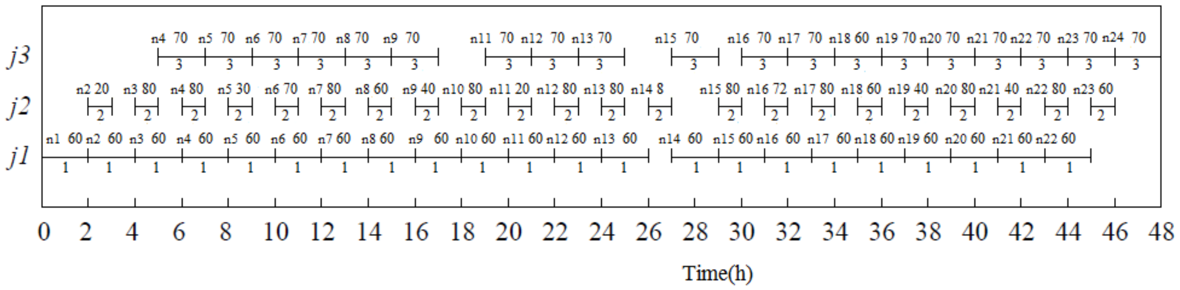


Fig. 3.2. Gantt chart for Example 3.1 without heat integration

3.3.1.2. Heat integrated mode

In direct heat integrated mode, the heat liberated in reaction task can be utilized in reboiler unit associated with distillation process. The reactor processing time when operated with heat integration is raised from 2 to 3 hr. Thus, the reactor and distillation units run in heat integrated mode with an offset of one hour with respect to the initial starting times. Further, the reactor in heat integration mode requires cooling water during its first hour of operation. Thereafter, the heat liberated during the reaction is exchanged with the reboiler of the distillation column.

For the optimal objective value of 3644.4, the proposed model requires 27 events and 104 binary variables whereas Chen and Chang (2009) model require 33 time points and 244 binary variables. An amount of 3.6 tons of hot utility is required for standalone distillation task and 7.2 tons of cooling water are required for standalone and first hour of integrated reaction task. The optimal Gantt chart for this case is shown in Fig. 3.3.

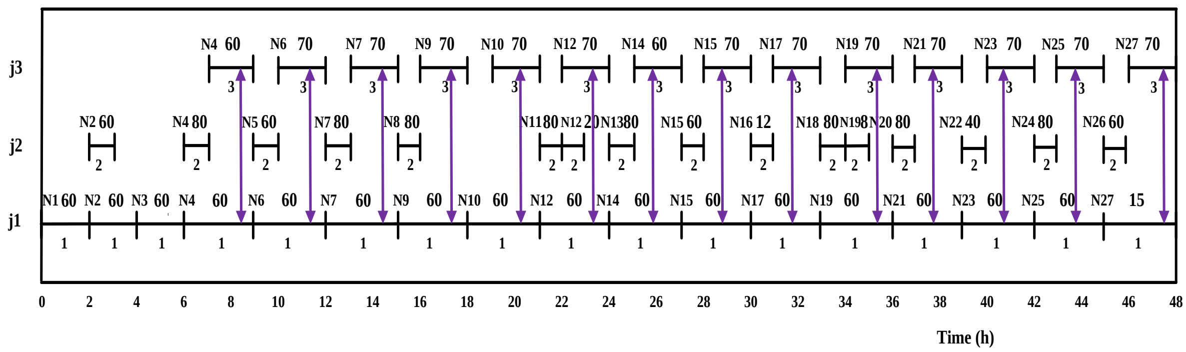


Fig. 3.3. Gantt chart for Example 3.1 with heat integration

From the Gantt chart it can be observed that the first three batches in reactor are operating in standalone mode. The rest of the batches are operating in a heat integrated mode as both the reaction and distillation tasks are taking place over the same time interval. The heat integrated process operation resulted in a better objective value due to the reduction in utility consumption as compared to the standalone process.

3.3.2. Example 3.2

Mazoji (2006) first presented this industrial example. The reactors R1 and R2 are used to handle reaction-1 where the two raw materials namely S1 and S9 are converted to intermediate S2. The reactors R3 and R4 are used to process the intermediates S2 and S3. The monosodium salt solution S4 obtained from reaction-3 is sent through the settlers for removing the solid byproduct S8. The excess water present in the resulted solid free monosodium salt solution is removed by using evaporators EV1 and EV2. Fig. 3.4 describes the production process using STN representation. The required process data is presented in Table 3.3. The selling price of the product (S6) is 100 rcu / ton and the cooling water cost is 8 rcu / ton and that of steam is 15 rcu / ton. The requisite heating load for evaporation is 4 ton and cooling load for reaction-2 is 5 ton. Therefore, in the presence of heat integration, the reaction-2 requires 1 ton of external cooling utility. In order to facilitate energy transfer, it is assumed that minimum ΔT is maintained between the hot and cold streams throughout the heat exchanger. The example is solved with the objective of profit maximization considering 15 hours time horizon.

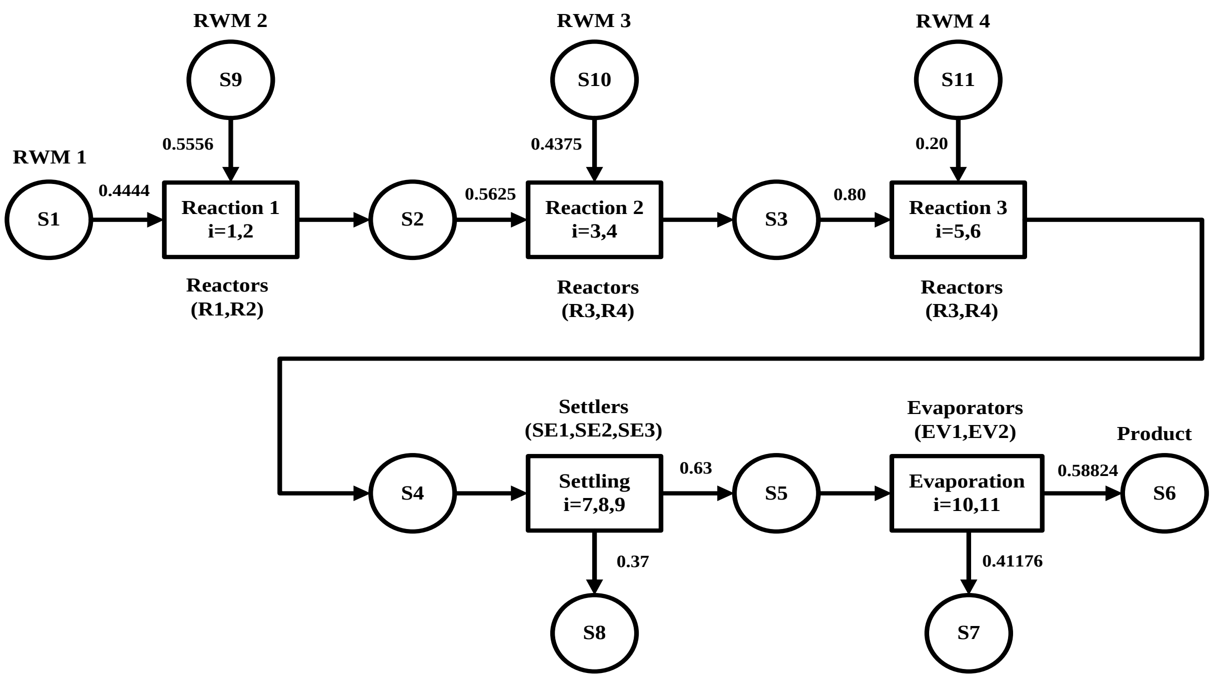


Fig. 3.4. STN for Example 3.2

Table 3.3. Data for Example 3.2

Task(i)	Unit (j)	Processing time	Capacity	States	Initial Amount	Storage Capacity
Reaction1	Reactor(R1)	2	8	S1	UL	UL
Reaction1	Reactor(R2)	2	8	S2	0	100
Reaction2	Reactor(R3)	3	8	S3	0	100
Reaction3	Reactor(R3)	1	8	S4	0	100
Reaction2	Reactor(R4)	3	8	S5	0	100
Reaction3	Reactor(R4)	1	8	S6	0	100
Settling	Settler(SE1)	1	8	S7	0	100
Settling	Settler(SE2)	1	8	S8	0	100
Settling	Settler(SE3)	1	8	S9	UL	UL
Evaporation	Evaporator(EV1)	3	8	S10	UL	UL
Evaporation	Evaporator(EV2)	3	8	S11	UL	UL

UL-Unlimited

3.3.2.1. Standalone mode

In standalone mode both hot and cold tasks are allowed to take place over different time intervals. The external utilities such as steam and water are used to meet the heating and cooling demands. The evaporation task utilizes steam as heating utility to maintain the desired temperature and reaction-2 utilizes water as cooling medium which removes the heat released from the exothermic reaction. The proposed model resulted in an optimal objective value of 1081.7 rcu and require 8 events. Whereas, Chen and Chang (2009) model reported the suboptimal objective of 1071 rcu. An amount of 16 tons of steam and 20 tons of cooling water utilities are required. The computational results and model statistics are presented in Table 3.4. The Gantt chart for this case is shown in Fig. 3.5.

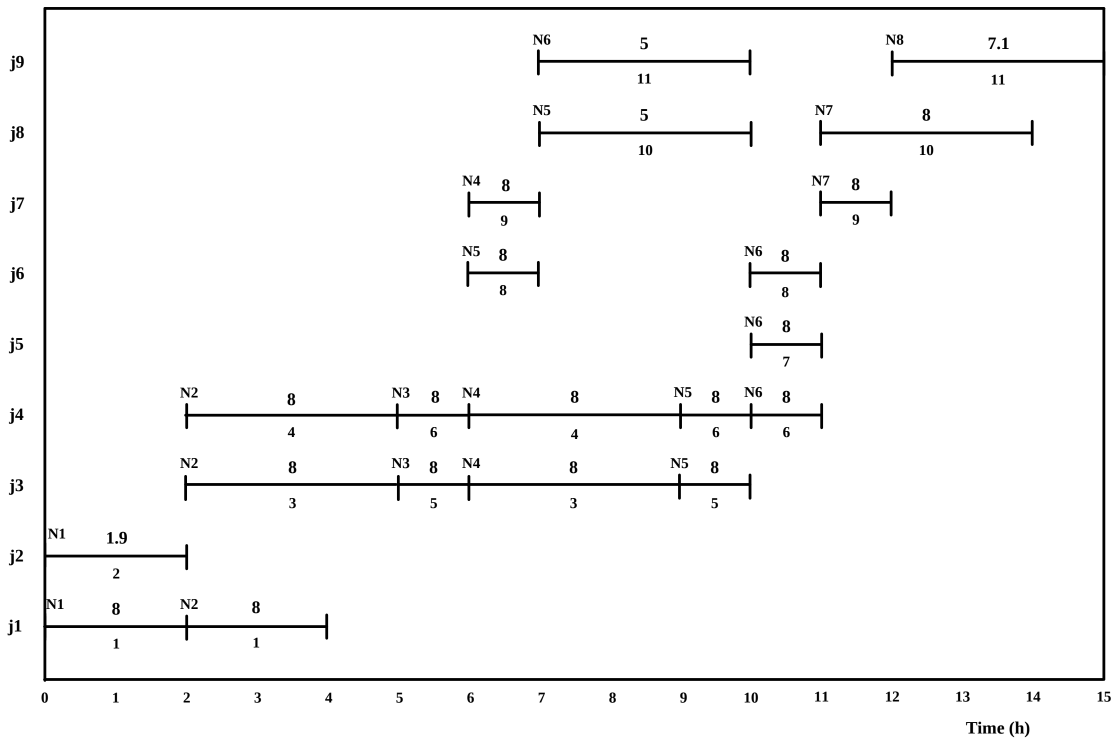


Fig. 3.5. Gantt chart for Example 3.2 without heat integration

Table 3.4. Computational results for Example 3.2

	Standalone		Heat integration	
Model used	Chen and Chang (2009)	The proposed USEB model	Chen and Chang (2009)	The proposed USEB model
Time points/Events	11	8	11	8
Objective value	1071	1081.7	1267	1267
RMILP	--[a]	1258.6	--[a]	1486.7
CPU time(sec)	64.67[b]	0.421	113.8[b]	0.202
Product(tons)	14.1	14.1	14.1	14.1
Steam(tons)	12	16	0	0
Cooling water(tons)	20	20	18	18
Binary variables	--[a]	88	--[a]	120
Continuous variables	--[a]	364	--[a]	492
Constraints	--[a]	820	--[a]	1324

[a]Not reported, [b]CPU time for Chen and Chang (2009) model is given for completeness only

3.3.2.2. Heat integrated mode

In the direct heat integration, both hot and cold tasks are integrated whenever they are active at the same time interval. In this case study, there is a possibility of heat integration between evaporation and reaction-2 tasks. The heat released from the exothermic reaction-2 is transferred to evaporation unit for maintaining the desired temperature. The additional cold utility required for reaction-2 in case of heat integration is met from external water utility. In the absence of heat integration, the evaporation and reaction-2 task will be active in standalone mode and external utilities are used to meet the demand. In standalone and heat integration modes the duration of both the tasks remains unaltered. The proposed model resulted in an optimal objective value of 1267 rcu and require 8 event points whereas Chen and Chang (2009) model requires 11 time points. The computational results are presented in Table 3.4 and the Gantt chart is shown in Fig. 3.6.

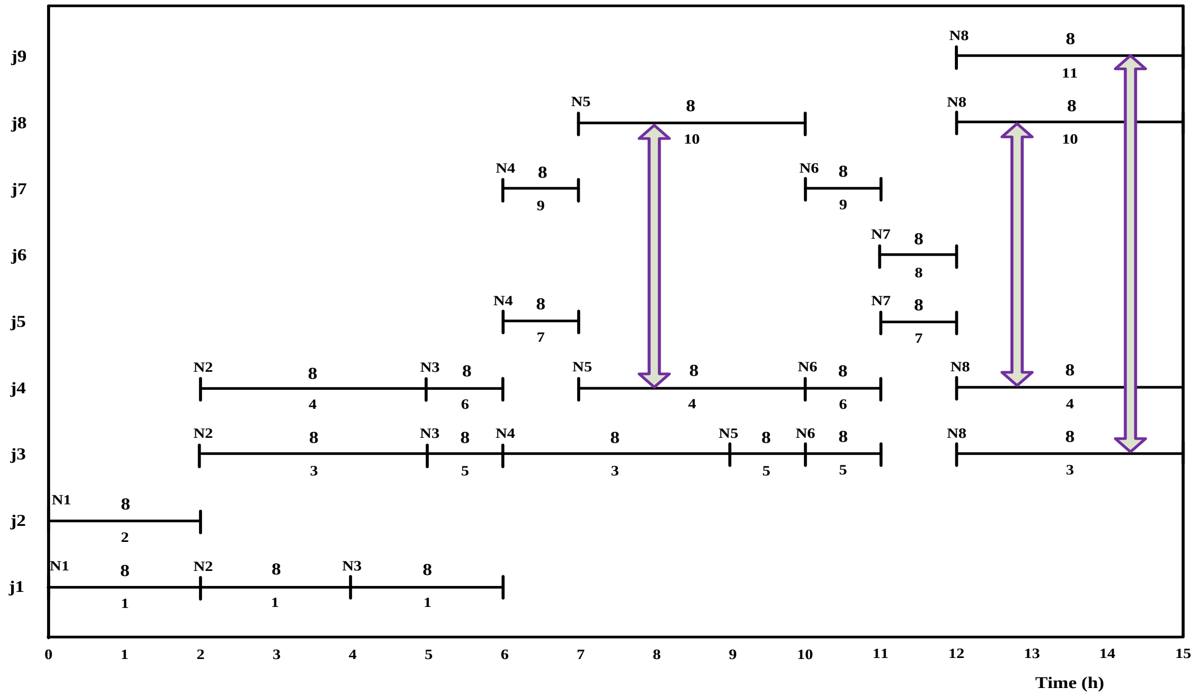


Fig. 3.6. Gantt chart for Example 3.2 with heat integration

3.4. Conclusions

Numerous robust batch plant scheduling models have been proposed in the literature. However, few models are extended to handle simultaneous heat integration. In this work, the robust scheduling model proposed by Vooradi and Shaik (2012) based on three index unit specific event formulation is extended to handle simultaneous scheduling and heat integration of batch plants. The bilinear terms in utility balance equations are linearized by using only two additional variables in Glover transformation. The proposed methodology is applicable for scheduling multiproduct and multipurpose batch plants. Compared to Chen and Chang (2009) model, the proposed formulation is found to be computationally superior and obtained optimal objective values with minimal number of event points, continuous variables and binary variables. In Example 3.2 without heat integration case study the proposed model reported better objective value of 1081.7 rcu as compared to the 1071 rcu reported in the literature.

CHAPTER 4

HEAT INTEGRATION AND CYCLIC SCHEDULING OF MULTIPURPOSE BATCH PLANTS USING THREE INDEX UNIT-SPECIFIC EVENT BASED MODEL

Heat integration and cyclic scheduling of multipurpose batch plants using three index unit-specific event based model

Process scheduling with a long time horizon always leads to large problem size, which is challenging to solve for global optimal solutions. The problem complexity further increases with the inclusion of additional tasks such as heat integration, water integration, material transfers and shared storage. Cyclic scheduling can be a potential option to handle the long time horizon scheduling problems. In cyclic scheduling, the longer time horizon is divided into cycles of equal time interval, thereby reducing the overall size of the problem. Extensive studies were available in literature for the handling of batch process scheduling with heat integration. Limited studies (Chen and Chang (2009); Stamp and Majozi (2017)) have embedded the concept of heat integration with cyclic scheduling to reduce the complexity while solving large-scale problems. Cyclic scheduling and heat integration has a significant scope for further study by effectively handling different cyclic scheduling and direct heat integration features.

To meet the objective 2.5.2 defined in chapter 2, a novel unified three index unit-specific event-based mathematical formulation is presented for cyclic scheduling of multipurpose batch plants. The unified framework reduces to a simple case in the absence of cyclic scheduling. The task extending to the next cycle is integrated with the short term scheduling constraints using the active task concept. Further, the framework is also extended for simultaneous cyclic scheduling and heat integration of multipurpose batch plants. The computational performance of the unified framework is evaluated with benchmark examples taken from the literature.

4.1. Problem statement

The problems on cyclic scheduling and cyclic scheduling with simultaneous heat integration are considered in this chapter. The data given for the case of cyclic scheduling is as follows: (i) process and production data, duration of the task, consumption/production coefficients for resources, time horizon, product recipes, raw materials cost, selling price of final products and cost incurred on operations (operating cost) (ii) data related to amount of heat and cold utilities required and associated costs are specified while handling simultaneous heat integration. The overall objective of this study is to maximize the profit per hour which is represented as the difference between total revenue from the products and utility cost. The objective function is sensitive to the following key decision variables: cycle time, utility requirements, task allocations and sequence, task start and end times and batch processing amounts.

The following assumptions are considered: negligible material transfer times, no unit failures, heat exchanger capital cost is not considered in profit maximization, batch processing time is linearly related with batch size, pre-processing material waiting is not allowed, the total time horizon is very long as compared with derived cyclic schedule, and initial & final periods are not optimized.

4.2. Mathematical formulation

The proposed formulation consists of a novel unified mathematical model which can be used for short term and cyclic scheduling of batch processes. Further, the unified model is also extended to handle heat integration. The unified model can be applied to both multiproduct and multipurpose batch processes with variable batch sizes. This unified model uses STN representation and consists of allocation, capacity, material balance, duration, sequencing, storage and utility-related constraints. The unified model is systematically explained in the following subsections 4.2.1 and 4.2.2. The newly proposed mathematical equations are presented in these subsections. The constraints (3.2), (3.5), (3.8) and (3.10) from Chapter 3 are directly adopted here as they are similar in nature.

4.2.1. Cyclic scheduling of batch processes

In this section, novel model equations are proposed for short term and cyclic scheduling of batch processes with an objective to maximize profit per hour. Optimal cycle time (H) is considered as a positive real variable and has been calculated from the specified cycle time range. The tasks which are continuing to the next cycle are modeled as active tasks at the last event and may extend to the beginning of the first event in the same cycle.

4.2.1.1. Objective Function

The cyclic scheduling objective function shown in constraint (4.1) represents the average profit per hour. The optimal cycle time is a variable and has been calculated from the specified cycle time horizon range.

$$Maxprofit = \sum_{S\in S^p} price(s)\left(\sum_{n1=N} ST(s,n1) + \sum_{i\in I_s^p} \rho_{is} \sum_{\substack{n2\in N \\ n1-\Delta n\leq n2\leq n1}} b(i,n2,n1)\right)\Big/H, \quad (4.1)$$

4.2.1.2. Allocation Constraints

Allocation constraint ensures that at the most one task can be active at an event point in any equipment. A single unified allocation constraint (4.2) can take care of the active task phenomena (Vooradi and Shaik (2012)) for the batch plants with and without cyclic scheduling.

$$\sum_{i\in I_j} \sum_{\substack{n2\in N \\ n1-\Delta n\leq n2\leq n1}} \sum_{\substack{n3\in N \\ n2\leq n3\leq n2+\Delta n}} w(i,n2,n3) + \sum_{i\in I_j} \sum_{\substack{n^a=n1 \\ n^a\leq \Delta n}} \sum_{\substack{n2\in N \\ N+n^a-\Delta n\leq n2\leq N}}$$

$$\sum_{\substack{n3 \in N \\ n^a \leq n3 \leq n2+\Delta n-N}} w(i,n2,n3) + \sum_{i \in I_j} \sum_{\substack{n^a = n1 \\ n^a \geq N-\Delta n+1}} \sum_{\substack{n2 \in N \\ n^a-\Delta n \leq n2 \leq n^a \\ n2 \geq N-\Delta n+1}} \sum_{\substack{n3 \in N \\ n3 \leq n2+\Delta n-N}} w\ (i,n2,n3) \leq 1,$$

$$\forall\ j \in J, n1 \in N \tag{4.2}$$

4.2.1.3. Capacity constraints

Constraint (4.3) enforces the batch size of the task *i* must be within the minimum and maximum capacity, if it is active and extended to the next cycle. Similarly, the constraint (3.2) can be used for the tasks which are starting and ending in the same cycle.

$$B_i^{min} w(i,n1,n2) \leq b(i,n1,n2) \leq B_i^{max} w(i,n1,n2),$$

$$\forall\ i \in I, n1, n2 \in N, B_i^{min}, n1 \geq N-\Delta n+1, n2 \leq n1+\Delta n-N, \Delta n > 0 \tag{4.3}$$

4.2.1.4. Material balances

Constraint (4.4) handles the material balance for all the states at the events *n*1>1. This unified constraint implies the consumption and/or production tasks that may extend to the next cycle. Here, the parameters I_s^p and I_s^c represent the fraction of state *s* produced and consumed by the task *i* respectively.

$$ST(s,n1) = ST(s,n1-1) + \sum_{i \in I_s^p} \rho_{is} \sum_{\substack{n2 \in N \\ n1-1-\Delta n \leq n2 \leq n1-1}} b(i,n2,n1-1) + \sum_{i \in I_s^p} \rho_{is} \sum_{\substack{n^a \in N \\ n^a = n1 \\ 1 \leq n^a \leq \Delta n+1}}$$

$$\sum_{\substack{n2 \in N \\ n2 \geq N+n^a-1-\Delta n}} b(i,n2,n1-1) + \sum_{i \in I_s^c} \rho_{is} \sum_{\substack{n2 \in N \\ n1 \leq n2 \leq n1+\Delta n}} b(i,n1,n2) + \sum_{i \in I_s^c} \rho_{is} \sum_{\substack{n^a \in N \\ n^a = n1 \\ n^a > N-\Delta n}}$$

$$\sum_{\substack{n2 \in N \\ n2 \leq n^a+\Delta n-N}} b(i,n^a,n2), \qquad \forall\ s \in S, n1 \in N, n1 > 1 \tag{4.4}$$

Equation (4.5) handles the material balance for the intermediate and raw material states at the first event. The Equations (4.4) and (4.5) will reduce to the simple material balance equations in the absence of cyclic scheduling.

$$ST(s,n1) = ST_0(s) + ST(s,N) + \sum_{i \in I_s^p} \rho_{is} \sum_{\substack{n2 \in N \\ n2 \geq N-\Delta n}} b(i,n2,N) + \sum_{i \in I_s^c} \rho_{is} \sum_{\substack{n2 \in N \\ n1 \leq n2 \leq n1+\Delta n}} b(i,n1,n2),$$

$$\forall\ s \in S^{IN} \cup S^R, n1 \in N, n1 = 1, \Delta n > 0 \tag{4.5}$$

4.2.1.5. Duration constraints

If Δ*n* is 0, then the finishing time of task *i* at event *n*1 is equal to the sum of the starting time of task *i* at that event and duration of the task as presented in constraint (3.5). If Δ*n* is nonzero, then the finishing time of task *i* at event point *n*2 is equal to the sum of the starting time of task *i* at event point *n*1 and duration of the task as presented in equations (4.6) to (4.9). Equations (4.7) and (4.9) are used to calculate the finishing time of the task, which extends to the next cycle. In the absence of cyclic scheduling, constraints (4.7) and (4.9) are redundant.

$$T^f(i,n2) \geq T^s(i,n1) + \gamma_i w(i,n1,n2) + \delta_i b(i,n1,n2),$$

$$\forall\ i \in I, n1, n2 \in N, n1 \leq n2 \leq n1 + \Delta n, n2 \leq N, \Delta n > 0 \quad (4.6)$$

$$T^f(i,n2) \geq T^s(i,n1) + \gamma_i w(i,n1,n2) + \delta_i b(i,n1,n2) - H,$$

$$\forall\ i \in I, n1, n2 \in N, n1 \geq N - \Delta n + 1, n2 \leq n1 + \Delta n - N, \Delta n > 0 \quad (4.7)$$

$$T^f(i,n2) \leq T^s(i,n1) + \gamma_i w(i,n1,n2) + \delta_i b(i,n1,n2) + M\big(1 - w(i,n1,n2)\big),$$

$$\forall\ i \in I, n1, n2 \in N, n1 \leq n2 \leq n1 + \Delta n, n2 \leq N, \Delta n > 0 \quad (4.8)$$

$$T^f(i,n2) \leq T^s(i,n1) + \gamma_i w(i,n1,n2) + \delta_i b(i,n1,n2) - H + M\big(1 - w(i,n1,n2)\big),$$

$$\forall\ i \in I, n1, n2 \in N, n1 \geq N - \Delta n + 1, n2 \leq n1 + \Delta n - N, \Delta n > 0 \quad (4.9)$$

4.2.1.6. Sequencing constraints

The constraint (4.10) ensures that the finishing time of task *i* at last event should be less than or equal to the cycle length H.

$$T^f(i,n1) \leq H, \qquad \forall\ i \in I, n1 \in N, n1 = N \quad (4.10)$$

4.2.1.7. Same task in the same unit

The constraint (3.8) enforces that the starting time of task *i* at event point *n*1 + 1 must be greater than or equal to the finish time of the same task in the same unit at event point *n*. If the task *i* is active and continuing to the next event *n*1+1 or first event of the next cycle, the start time should be equal to finish time of task *i* at event *n*1 or the last event of the cycle respectively. Equations (4.11) and (4.12) ensure task continuity by enforcing the task *i* finish time at event *n* equals to start time at event *n*1+1. In this formulation, the continuity of the task which extend to next cycle is handled by representing the extending portion at the beginning of same cycle. Equations (4.11) and (4.12) ensure that the finish time of active task *i* at event N equals to start time of the first event.

$$T^s(i,n1+1) \leq T^f(i,n1) + M\left(1 - \sum_{\substack{n2 \in N \\ n1-\Delta n \leq n2 \leq n1}} \sum_{\substack{n3 \in N \\ n2 \leq n3 \leq n2+\Delta n}} w(i,n2,n3) - \sum_{\substack{n2, n^a \in N; n^a = n1 \\ N-\Delta n < n^a < N \\ n^a - \Delta n \leq n2 \leq n^a \\ n2 \geq N - \Delta n + 1}} \sum_{\substack{n3 \in N \\ n3 \leq n2 + \Delta n - N}} w(i,n2,n3) - \sum_{\substack{n2, n^a \in N; n^a = n1 \\ n^a \leq \Delta n \\ N + n^a - \Delta n \leq n2 \leq N}} \sum_{\substack{n3 \in N \\ n^a \leq n3 \leq n2 + \Delta n - N}} w(i,n2,n3)\right),$$

$$\forall\ i \in I, n1 \in N, n1 < N, \Delta n > 0 \quad (4.11)$$

$$T^s(i,n^a) \leq T^f(i,n1) - H + M\left(1 - \sum_{\substack{n2 \in N \\ N-\Delta n+1 \leq n2 \leq n1}} \sum_{\substack{n3 \in N \\ n3 \leq n2 + \Delta n - N}} w(i,n2,n3)\right),$$

$$\forall\ i \in I, n1 \in N, n1 = N, \Delta n > 0 \quad (4.12)$$

4.2.1.8. Different tasks in the same unit

The starting time of task i at event point $n1 + 1$ should be greater than or equal to finishing time of a different task in the same unit at event point n as shown in the constraint (3.10).

4.2.1.9. Different tasks in different units

$$T^s(i,n1+1) \geq T^f(i1,n1) - M\left(1 - \sum_{\substack{n2\in N\\ n1-\Delta n\leq n2\leq n1}} w(i1,n2,n1) - \sum_{\substack{n2,n^a\in N;n^a=n1\\ n^a\leq \Delta n\\ N+n^a-\Delta n\leq n2\leq N}} w(i1,n2,n1)\right),$$

$$\forall\ s\in S, i\in I_j, i1\in I_{j1}, i\in I_s^c, i1\in I_s^p, i\neq i1, j, j1\in J, j\neq j1, n1\in N, n1\leq N \qquad (4.13)$$

Constraint (4.13) relates the different tasks (i,$i1$) occurring in different units (j,$j1$) and avoids the real-time material flow violations. The starting time of the consuming task at next event $n1$+1 is enforced to be greater than the finish time of the producing task at the current event $n1$.

4.2.1.10. Different Storage policies

Constraint (4.14) along with constraint (4.13) imposes no-wait condition required for different tasks occurring in different units that produce or consume the same intermediate state having the restriction of either zero-wait policy (ZW) or no intermediate storage (NIS) or dedicated finite intermediate storage (DFIS) cases.

$$T^s(i,n1+1) \leq T^f(i1,n1) + M\left(2 - \sum_{\substack{n2\in N\\ n2\leq n1\leq n2+\Delta n}} w(i1,n2,n1) - \sum_{\substack{n2,n^a\in N;n^a=n1\\ n^a\leq \Delta n\\ N+n^a-\Delta n\leq n2\leq N}} w(i1,n2,n^a)\right.$$
$$\left. - \sum_{\substack{n2\in N\\ n1+1\leq n2\leq n1+1+\Delta n}} w(i,n1+1,n2) - \sum_{\substack{n2\in N\\ n1+1>N-\Delta n\\ n2\leq n1+1+\Delta n-N}} w(i,n1+1,n2)\right),$$

$$\forall\ s\in S^{dfis}, S^{nis}, S^{zw}, i\in I_j, i1\in I_{j1}, i\in I_s^c, i1\in I_s^p, i\neq i1, j, j1\in J, j\neq j1, n1\in N, n1< N \qquad (4.14)$$

For handling finite dedicated intermediate storage the following constraint (4.15) is used to avoid real-time violations in addition to the constraint (4.14).

$$T^f(i1,n1) \geq T^s(i,n1) - M\left(1 - \sum_{\substack{n2\in N\\ n1-\Delta n\leq n2\leq n1}} w(i1,n2,n1) - \sum_{\substack{n2\in N\\ n2\geq N-\Delta n+n3}} \sum_{\substack{n3\in N\\ n3\leq \Delta n\\ n3\leq n1}} w(i1,n2,n3)\right),$$

$$\forall\ s\in S^{fis}, i\in I_j, i1\in I_{j1}, i\in I_s^c, i1\in I_s^p, i\neq i1, j, j1\in J, j\neq j1, n1\in N, n1\leq N \qquad (4.15)$$

4.2.1.11. Merits of the proposed formulation:

In this section, the modelling advantages of the proposed framework compared to Wu and Ierapetritou (2004) model are presented.

- The framework uses three index binary ($w(i,n1,n2)$) and continuous ($b(i,n1,n2)$) variables. These variables can easily handle the task continuity over multiple events and have the advantage (Shaik and Floudas (2009)) in finding the optimal solution. The computational results of Example 4.1 for cycle time range 200-240 h highlights the advantage of task continuing over multiple events.
- The Wu and Ierapetritou (2004) model utilizes the first event point to track the inventory of intermediates available at the cycle starting time. The proposed formulation handles this with an active task concept and without the need of an extra event point. Therefore, the proposed model consistently requires at least one event less than the Wu and Ierapetritou (2004) model.
- The storage of intermediate states and real time storage violations are monitored using two auxiliary constraints (4.14) and (4.15). Wu and Ierapetritou (2004) model imposes maximum limit on the amount of material stored at an event point. However, this approach can result in storage violation on a real time horizon (Shaik and Floudas (2008)).
- The proposed formulation integrates the cyclic scheduling and process scheduling model equations on a unified framework, whereas Wu and Ierapetritou (2004) model appended cyclic scheduling constraints to short term scheduling model. Hence, the size of the proposed model (in terms of model equations, continuous variables and binary variables) will be considerably less than Wu and Ierapetritou (2004) model.

4.2.2. Cyclic scheduling with heat integration of batch plants

The unified model proposed in section 4.2.1 for short term and cyclic scheduling of batch plants has been extended to handle the direct heat integration. In heat integration, the active hot and cold tasks are enforced to start at the same time interval to facilitate the direct heat transfer.

4.2.2.1. Objective function

The linear objective function presented in equation (4.16) evaluates the net profit by deducting the external utility costs from product revenue. Here, the profit is evaluated at specified cycle time. The objective function (4.17) represents the average profit per hour, where the cycle time is considered as a variable and will be calculated from the specified time horizon range.

$$Maxprofit\ \ Z = \sum_{s \in S^p} price(s) \left(\sum_{n1=N} ST(S,n1) + \sum_{i \in I_s^p} \rho_{is} \sum_{\substack{n2 \in N \\ n1-\Delta n \le n2 \le n1}} b(i,n2,n1) \right)$$

$$- \sum_{i \in I_h} \sum_{n1=1}^{N} \big(c_{uh} qhi(i,n1)\big) - \sum_{i \in I_c} \sum_{n1=1}^{N} \big(c_{uc} q(i,n1)\big), \tag{4.16}$$

$$Objective\ function = \frac{Maxprofit}{H} \tag{4.17}$$

4.2.2.2. Task integration

Constraint (4.18) and (4.19) ensure that one to one integration of heating task with cooling task if both tasks are active. The binary variable *x*(*i*,*i1*,*n1*) value of one at event *n1* represents task *i* which require heating is integrated with task *i1* which require cooling.

$$\sum_{i1 \in I_c} x(i,i1,n1) \le \sum_{\substack{n2 \in N \\ n1 \le n2 \le n1+\Delta n}} w(i,n1,n2) + \sum_{\substack{n^a \in N \\ n^a = n1 \\ n^a > N-\Delta n}} \sum_{\substack{n2 \in N \\ n2 \le n^a + \Delta n - N}} w(i,n1,n2),$$

$$\forall \ \ i \in I_h, i \neq i1, n1 \in N \tag{4.18}$$

$$\sum_{i \in I_h} x(i,i1,n1) \le \sum_{\substack{n2 \in N \\ n1 \le n2 \le n1+\Delta n}} w(i1,n1,n2) + \sum_{\substack{n^a \in N \\ n^a = n1 \\ n^a > N-\Delta n}} \sum_{\substack{n2 \in N \\ n2 \le n^a + \Delta n - N}} w(i1,n1,n2),$$

$$\forall \ \ i1 \in I_c, i \neq i1, n1 \in N \tag{4.19}$$

4.2.2.3. Utility constraints

Constraint (4.20) calculates the amount of hot utility required for task *i*, if it is active in standalone mode. Constraint (4.21) finds the hot utility required for task *i*, when it operates in heat integrated mode.

$$q(i,n) = \alpha_i \left(\sum_{\substack{n2 \in N \\ n1 \le n2 \le n1+\Delta n}} w(i,n1,n2) + \sum_{\substack{n^a \in N \\ n^a = n1 \\ n^a > N-\Delta n}} \sum_{\substack{n2 \in N \\ n2 \le n^a + \Delta n - N}} w(i,n1,n2) - \sum_{i1 \in I_c} x(i,i1,n1) \right)$$

$$+\beta_i \left(1 - \sum_{i1 \in I_c} x(i,i1,n1) \right) \left(\sum_{\substack{n2 \in N \\ n1 \le n2 \le n1+\Delta n}} b(i,n1,n2) + \sum_{\substack{n^a \in N \\ n^a = n1 \\ n1 > N-\Delta n}} \sum_{\substack{n2 \in N \\ n2 \le n^a + \Delta n - N}} b(i,n1,n2) \right),$$

$$\forall \ \ i \in I_h, i \neq i1, n1 \in N \tag{4.20}$$

$$q1(i,n1) = \alpha_i' \left(\sum_{i1 \in I_c} x(i,i1,n1) \right) + \beta_i' \sum_{i1 \in I_c} x(i,i1,n1) \left(\sum_{\substack{n2 \in N \\ n1 \le n2 \le n1+\Delta n}} b(i,n1,n2) + \right.$$

$$\sum_{\substack{n^a \in N \\ n^a = n1 \\ n^a > N - \Delta n}} \sum_{\substack{n2 \in N \\ n2 \le n^a + \Delta n - N}} b(i, n1, n2) \Bigg), \quad \forall \;\; i \in I_h, i \neq i1, n1 \in N \qquad (4.21)$$

Similar to the constraints (4.20) and (4.21), the constraints (4.22) and (4.23) calculate the amount of cold utility required for the active task $i1$ in standalone and heat integrated modes respectively.

$$q(i1, n1) = \alpha_{i1} \Bigg(\sum_{\substack{n2 \in N \\ n1 \le n2 \le n1 + \Delta n}} w(i1, n1, n2) + \sum_{\substack{n^a \in N \\ n^a = n1 \\ n^a > N - \Delta n}} \sum_{\substack{n2 \in N \\ n2 \le n1 + \Delta n - N}} w(i1, n1, n2)$$

$$- \sum_{i \in I_h} x(i, i1, n1) \Bigg) + \beta_i \Bigg(1 - \sum_{i \in I_h} x(i, i1, n1) \Bigg) \Bigg(\sum_{\substack{n2 \in N \\ n1 \le n2 \le n1 + \Delta n}} b(i1, n1, n2) +$$

$$\sum_{\substack{n^a \in N \\ n^a = n1 \\ n^a > N - \Delta n}} \sum_{\substack{n2 \in N \\ n2 \le n^a + \Delta n - N}} b(i, n1, n2) \Bigg), \quad \forall \;\; i1 \in I_c, i \neq i1, n1 \in N \qquad (4.22)$$

$$q1(i1, n1) = \alpha'_{i1} \Bigg(\sum_{i \in I_h} x(i, i1, n1) \Bigg) + \beta'_{i1} \sum_{i \in I_h} x(i, i1, n1) \Bigg(\sum_{\substack{n2 \in N \\ n1 \le n2 \le n1 + \Delta n}} b(i1, n1, n2) +$$

$$\sum_{\substack{n^a \in N \\ n^a = n1 \\ n^a > N - \Delta n}} \sum_{\substack{n2 \in N \\ n2 \le n1 + \Delta n - N}} b(i1, n1, n2) \Bigg), \quad \forall \;\; i1 \in I_c, i \neq i1, n1 \in N \qquad (4.23)$$

The bilinear terms *x(i,i1,n1)*b(i,n1,n2)* and *x(i,í1,n1)*b(i1,n1,n2)* used in utility balance equations are represented as *bh*(*i*,*i1*,*n1*) and *bc*(*i*,*i1*,*n1*) respectively. Using the Glover transformation these new variables are linearly defined. The constraints (4.24) to (4.27) complete the linear transformation of the above bilinear terms.

$$B_i^{min} x(i, i1, n1) \le bh(i, i1, n1) \le B_i^{max} x(i, i1, n1), \quad \forall \;\; i \in I_h, i1 \in I_c, n1 \in N \qquad (4.24)$$

$$B_{i1}^{min} x(i, i1, n1) \le bc(i, i1, n1) \le B_{i1}^{max} x(i, i1, n1), \quad \forall \;\; i \in I_h, i1 \in I_c, n1 \in N \qquad (4.25)$$

$$\sum_{\substack{n2 \in N \\ n1 \le n2 \le n1 + \Delta n}} b(i, n1, n2) + \sum_{\substack{n^a \in N \\ n^a = n1 \\ n^a > N - \Delta n}} \sum_{\substack{n2 \in N \\ n2 \le n1 + \Delta n - N}} b(i, n1, n2) - B_i^{max} \big(1 - x(i, i1, n1)\big)$$

$$\le bh(i, i1, n1) \le \sum_{\substack{n2 \in N \\ n1 \le n2 \le n1 + \Delta n}} b(i, n1, n2) + \sum_{\substack{n^a \in N \\ n^a = n1 \\ n^a > N - \Delta n}} \sum_{\substack{n2 \in N \\ n2 \le n^a + \Delta n - N}} b(i1, n1, n2),$$

$$\forall \;\; i \in I_h, i1 \in I_c, n1 \in N \qquad (4.26)$$

$$\sum_{\substack{n2\in N\\ n1\le n2\le n1+\Delta n}} b(i1,n1,n2) + \sum_{\substack{n^a\in N\\ n^a=n1\\ n^a>N-\Delta n}} \sum_{\substack{n2\in N\\ n2\le n^a+\Delta n-N}} b(i1,n1,n2) - B_{i1}^{max}\big(1-x(i,i1,n1)\big)$$

$$\le bc(i,i1,n1) \le \sum_{\substack{n2\in N\\ n1\le n2\le n1+\Delta n}} b(i1,n1,n2) + \sum_{\substack{n^a\in N\\ n^a=n1\\ n^a>N-\Delta n}} \sum_{\substack{n2\in N\\ n2\le n^a+\Delta n-N}} b(i1,n1,n2),$$

$$\forall \;\; i\in I_h, i1\in I_c, n1\in N \tag{4.27}$$

Constraints (4.28) and (4.29) ensure that integrated heating and cooling tasks must start at the same time.

$$T^s(i,n1) \ge T^s(i1,n1) - M\big(1-x(i,i1,n1)\big), \qquad \forall \;\; i\in I_h, i1\in I_c, n1\in N \tag{4.28}$$

$$T^s(i,n1) \le T^s(i1,n1) + M\big(1-x(i,i1,n1)\big), \qquad \forall \;\; i\in I_h, i1\in I_c, n1\in N \tag{4.29}$$

Constraints (4.30) to (4.35) are proposed to calculate the duration of heating and cooling tasks. Constraints (4.30) and (4.31) are used to calculate the task duration at event $n1$ where Δn is equal to zero. If Δn is nonzero, then the task may continue to next event and/or cycle. Thus, task i finishing at event $n1$ is equal to task i starting at same event $n1$ plus the task duration as calculated using constraints (4.32) to (4.35). The batch size-independent processing times are considered and modeled for heat integrated tasks.

$$T^f(i,n1) = T^s(i,n1) + \gamma_i\left(w(i,n1,n1) - \sum_{i1\in I_c} x(i,i1,n1)\right) + \gamma_i' \sum_{i1\in I_c} x(i,i1,n1),$$

$$\forall \;\; i\in I_h, i\ne i1, n1\in N, \Delta n = 0 \tag{4.30}$$

$$T^f(i1,n1) = T^s(i1,n1) + \gamma_{i1}\left(w(i1,n1,n1) - \sum_{i\in I_h} x(i,i1,n1)\right) + \gamma_{i1}' \sum_{i\in I_h} x(i,i1,n1)\,,$$

$$\forall \;\; i1\in I_c, i\ne i1, n1\in N, \Delta n = 0 \tag{4.31}$$

$$T^f(i,n1) \ge T^s(i,n1) + \gamma_i\left(w(i,n1,n2) - \sum_{i1\in I_c} x(i,i1,n1)\right) + \gamma_i' \sum_{i1\in I_c} x(i,i1,n1)$$

$$-M\big(1-w(i,n1,n2)\big) - H\left(\sum_{\substack{n^a\in N\\ n^a=n1\\ n^a>N-\Delta n}} \sum_{\substack{n^b\in N\\ n^b=n2\\ n^b\le n^a+\Delta n-N}} w\big(i,n^a,n^b\big)\right), \qquad \forall \;\; i\in I_h, i\ne i1, n1,$$

$$n2\in N, (n1\le n2\le n1+\Delta n, n2\le N)\cup(n1\ge N-\Delta n+1, n2\le n1+\Delta n-N), \Delta n>0 \tag{4.32}$$

$$T^f(i,n2) \le T^s(i,n1) + \gamma_i\left(w(i,n1,n2) - \sum_{i1\in I_c} x(i,i1,n1)\right) + \gamma_i' \sum_{i1\in I_c} x(i,i1,n1)$$

$$+M\big(1-w(i,n1,n2)\big)-H\left(\sum_{\substack{n^a\in N\\ n^a=n1\\ n^a>N-\Delta n}}\ \sum_{\substack{n^b\in N\\ n^b=n2\\ n^b\le n^a+\Delta n-N}} w\big(i,n^a,n^b\big)\right),\quad \forall\ \ i\in I_h, i\neq i1, n1,$$

$$n2\in N,(n1\le n2\le n1+\Delta n, n2\le N)\cup(n1\ge N-\Delta n+1, n2\le n1+\Delta n-N),\Delta n>0 \quad (4.33)$$

$$T^f(i1,n2)\ge T^s(i1,n1)+\gamma_{i1}\left(w(i1,n1,n2)-\sum_{i\in I_h}x(i,i1,n1)\right)+\gamma'_{i1}\sum_{i\in I_h}x(i,i1,n1)-$$

$$M\big(1-w(i1,n1,n2)\big)-H\left(\sum_{\substack{n^a\in N\\ n^a=n1\\ n^a>N-\Delta n}}\ \sum_{\substack{n^b\in N\\ n^b=n2\\ n^b\le n^a+\Delta n-N}} w\big(i1,n^a,n^b\big)\right),\forall\ \ i1\in I_c, i\neq i1, n1,$$

$$n2\in N,(n1\le n2\le n1+\Delta n, n2\le N)\cup(n1\ge N-\Delta n+1, n2\le n1+\Delta n-N),\Delta n>0 \quad (4.34)$$

$$T^f(i1,n2)\le T^s(i1,n1)+\gamma_{i1}\left(w(i1,n1,n2)-\sum_{i\in I_h}x(i,i1,n1)\right)+\gamma'_{i1}\sum_{i\in I_h}x(i,i1,n1)+$$

$$M\big(1-w(i1,n1,n2)\big)-H\left(\sum_{\substack{n^a\in N\\ n^a=n1\\ n^a>N-\Delta n}}\ \sum_{\substack{n^b\in N\\ n^b=n2\\ n^b\le n^a+\Delta n-N}} w\big(i1,n^a,n^b\big)\right),\quad \forall\ \ i1\in I_c, i\neq i1, n1,$$

$$n2\in N,(n1\le n2\le n1+\Delta n, n2\le N)\cup(n1\ge N-\Delta n+1, n2\le n1+\Delta n-N),\Delta n>0 \quad (4.35)$$

4.2.2.4. Merits of the proposed heat integration framework:

- Minimum number of bilinear terms are used in utility balance equations to linearize the model.
- The size of the proposed unit specific event based formulation will be less than the global event based model proposed by Chen and Chang (2009).

4.3. Computational case studies

Four examples are chosen from the literature to demonstrate the feasibility of the proposed model. These examples namely Motivating Example, Example 4.1, Example 4.2 and Example 4.3 are solved using GAMS 24.4.1/BARON to find the optimal cycle time and maximum profit per hour. Example 4.3 is also solved using GAMS 24.4.1/CPLEX to find the maximum profit in the specified cycle time. The desktop computer consisting of Intel Xeon E5-1607 3.00 GHz processor with 8 GB RAM and Windows 7 operating system is used as a computational resource. The computational results for the Wu and Ierapetritou (2004) & Chen and Chang (2009) models are taken directly from their papers; hence, CPU times for these two models are not directly compared here due to differences in hardware. In the proposed formulation, the minimum number of events and Δn required for obtaining the optimal objective value is estimated iteratively. The following computational scheme is used for solving examples: i) extraction of problem data in the form of sets, parameters, binary and continuous variables, ii) structure development in GAMS software by adding the model equations and problem data iii) solve the model using MINLP or MILP solver. The model gives infeasible or suboptimal solution for the event points less than the minimum number of events and Δn. As the number event points and/or Δn increases, the objective value improves and after some iterations, there will not be any improvement in the solution even at higher event points and Δn. The minimum number of events and Δn, where this optimal solution is resulted will be considered as number of events and Δn required.

4.3.1. Motivating Example

The motivating example is chosen from Wu and Ierapetritou (2004). The STN representation shown in Fig. 4.1 describes all the physical and chemical processes involved in the production scheme. In this flowsheet, two products using five processing stages: heating, Reaction1, Reaction2, Reaction3, and separation through which the raw materials and intermediates are processed. Table 4.1 shows the necessary data needed for the process. The procedure adopted in evaluating objectives such as optimal schedule and cycle length is as follows. The entire cycle time range of 2 to 24 h is truncated into cycles of several subranges like 2-6, 6-10, up to 24 h and each of the cycles is solved independently.

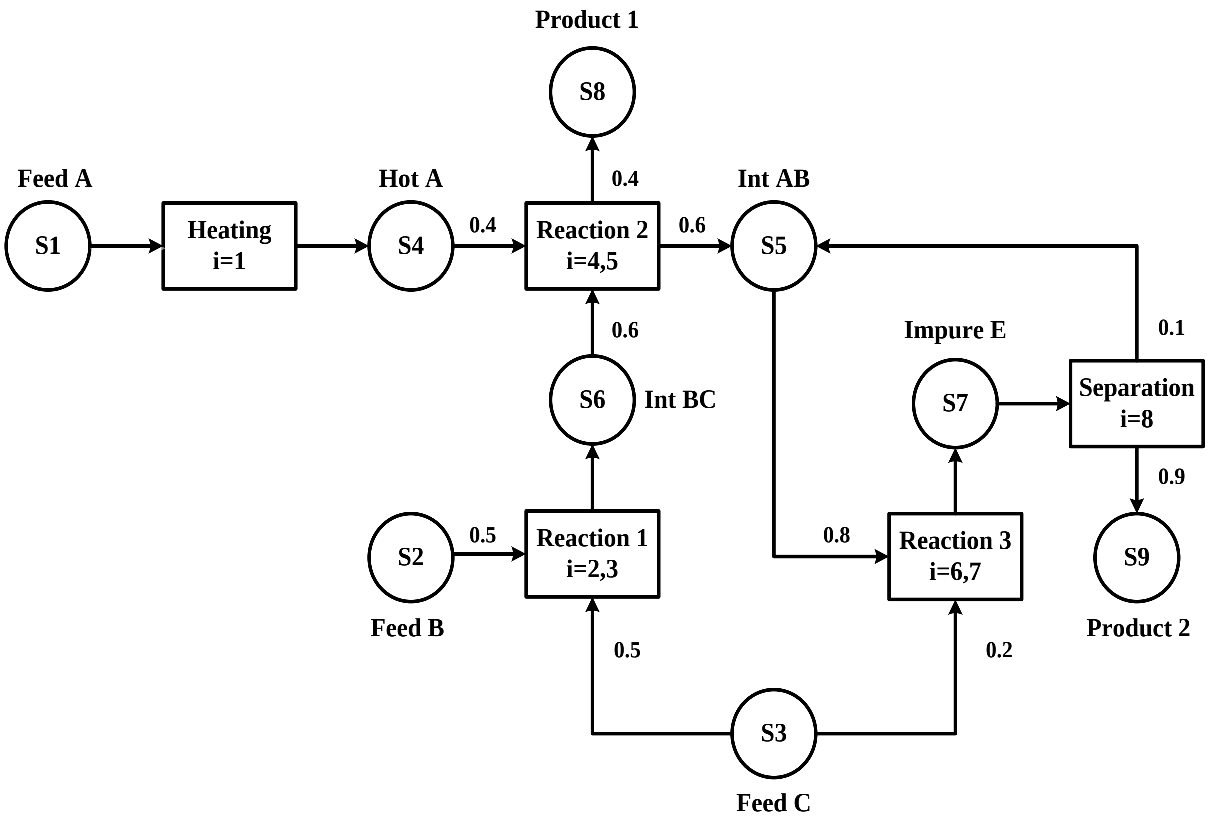


Fig. 4.1. STN representation for Motivating Example

Table 4.1. Data for Motivating Example

Unit(j)	Task(i)	Min. Batch size (mu)	Max. Batch size (mu)	Constant batch Processing time (α_i)	Variable batch Processing time (β_i)
Heater	Heating(i=1)	0	100	0.667	0.00667
Reactor 1	Reaction 1(i=2)	0	50	1.334	0.02664
Reactor 2	Reaction 1(i=3)	0	80	1.334	0.01665
Reactor 1	Reaction 2(i=4)	0	50	1.334	0.02664
Reactor 2	Reaction 2(i=5)	0	80	1.334	0.01665
Reactor 1	Reaction 3(i=6)	0	50	0.667	0.01332
Reactor 2	Reaction 3(i=7)	0	80	0.667	0.008325
Separator	Separation(i=8)	0	200	1.3342	0.00666
States	**Price ($/mu)**	**Initial Amount (mu)**		**Storage capacity (mu)**	
S1-S3	0	UL		UL	
S4	0	0		100	
S5	0	0		200	
S6	0	0		150	
S7	0	0		200	
S8	10	0		UL	
S9	10	0		UL	

UL=Unlimited

The advantages of adopting this kind of approach are (i) usage of sufficient number of event points and Δn for each of the sub-cycle to find the optimal solution (ii) possibility of creating more scheduling alternatives with various cycle lengths based on work shift constraints incorporation and consideration. The computational results presented in Table 4.2 show the effect of number of events and Δn on the objective value for motivating example at cycle time range 6h – 10h. Better objective function value is obtained as the number of event points increase and optimal solution is found at four event points and Δn is equal to zero. The model gives the same optimal result even at higher event points and Δn. As the number of event points and Δn increases, the model size (number of variables and equations) increases, which ultimately results in computational burden. Hence, the minimum number of events and Δn required for this case are estimated as 4 and 0 respectively. Estimation of optimal number of event points using iterative methods is time consuming. However, this formulation can adopt the alternate methodology presented in Li and Floudas (2010) for determining the optimal event points.

The computational results for motivating example at different cycle time ranges are presented in Table 4.3 and the results show that the proposed mathematical formulation requires fewer event points in obtaining the optimal objective value as compared to the Wu and Ierapetritou (2004) model. For the cycle time range 6-10 h the proposed model reported better optimal cycle time as compared with Wu and Ierapetritou (2004) model for the same profit per hour. The Gantt chart for a cycle time of 6-10 h is shown in Fig. 4.2. In the Gantt chart, the x-axis represent real time horizon in hours and y-axis represent processing units. The processing tasks are highlighted by using three identifiers including task number at the bottom, batch processing amount at the top and event number on the left side. The Gantt chart can be read with the help of these three identifiers. For instance, in Fig. 4.2 at event n1 the task four is active in Reactor 1 and it is processing 50 mass units (mu) of material in the duration of 2.66 hours. For cycle time ranges 14-18 and 18-21 the model reported better objective values as compared to Wu and Ierapetritou (2004) model. The Gantt chart for the cycle time range 18-21 h is presented in Fig. 4.3. The RMINLP column in the Table 4.2 represents solution to the Relaxed Mixed Integer Non-Linear Programing problem. The relaxed model types RMIP and RMINLP solve the problem in same way as MIP and MINLP, but relax the discrete requirement of the discrete variables. This means that integer and binary variables may assume any values between their bounds. For instance, the binary variable may assume any value between 0 and 1. The model is considered to be well defined and computationally superior, if the optimal solution is close to the relaxed solution.

Table 4.2. Computational results for motivating example at different event points for cycle time range 6h – 10h

Events	Δn	MINLP (Profit/h)	RMINLP (Profit/h)	Optimal cycle time (h)	CPU time (s)	Binary variables	Continuous variables	Constraints
1	0	0	0	6.000	0.060	8	29	40
2	0	182.222	206.589	6.000	0.100	16	69	119
2	1	182.222	206.589	6.000	0.180	32	85	208
3	0	272.234	284.532	6.526	0.490	24	102	198
3	1	272.234	290.581	6.526	2.680	48	126	318
3	2	272.234	292.260	6.526	3.300	72	150	420
4	0	272.309	296.569	7.743	0.820	32	135	277
4	1	272.309	385.108	7.743	5.750	64	167	437
4	2	272.309	406.607	7.743	7.950	96	199	542
4	3	272.309	322.695	7.743	7.200	128	231	680
5	0	272.309	315.798	7.743	14.430	40	168	356
5	1	272.309	335.220	7.743	46.390	80	208	556
5	2	272.309	331.265	7.743	125.090	120	248	676
5	3	272.309	328.680	7.743	80.020	160	288	826
6	0	272.309	429.883	7.743	51.720	48	201	435
6	1	272.309	431.355	7.743	1174.68	96	249	675
6	2	272.309	328.693	7.743	2049.89	144	297	819

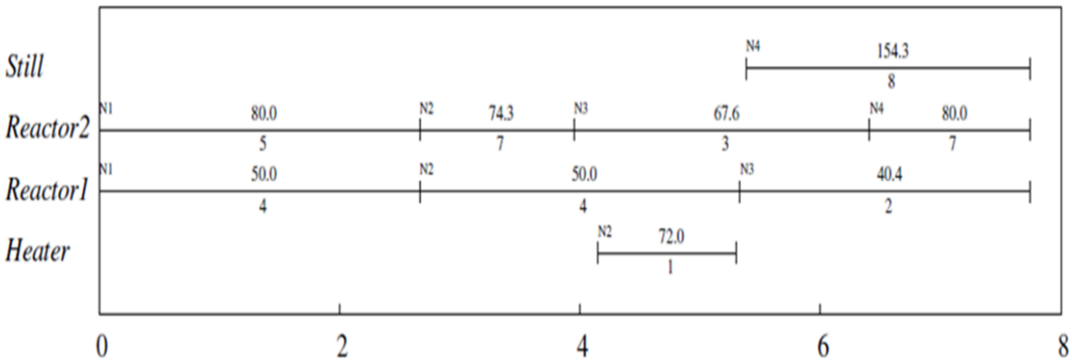


Fig. 4.2. Gantt chart for motivating example for cycle time range of 6-10 h

Table 4.3. Computational results for motivating example

Model	Cycle time range (h)	Events	MINLP (Profit/h)	RMINLP (Profit/h)	Optimal cycle time (h)	CPU time (s)	Binary variables	Continuous variables	Constraints
Wu & Ierapetritou	2-6	4	268.289	--[a]	5.094	2.86	48	299	530
This work	2-6	3	268.346	342.181	5.093	0.460	24	102	198
Wu & Ierapetritou	6-10	6	272.247	--[a]	9.036	512.00	--[a]	--[a]	--[a]
This work	6-10	4	272.309	296.569	7.743	0.790	32	135	277
Wu & Ierapetritou	10-14	7	273.801	--[a]	12.978	5365.74	--[a]	--[a]	--[a]
This work	10-14	6	273.864	302.572	12.975	159.400	48	201	435
Wu & Ierapetritou	14-18	9	276.447	--[a]	14.407	305.88	--[a]	--[a]	--[a]
This work	14-18	8	277.430	295.018	15.764	1268.63	64	267	593
Wu & Ierapetritou	18-21	11	277.363	--[a]	19.709	545.83	--[a]	--[a]	--[a]
This work	18-21	11	278.432	287.451	19.774	20000 [b,c]	88	366	830
Wu & Ierapetritou	21-24	12	279.029	--[a]	23.790	2884.41	--[a]	--[a]	--[a]
This work	21-24	11	279.097	286.054	23.784	20000 [b,d]	88	366	830

--[a] Not reported, [b] Resource limit reached, [c] Relative gap: 1.35%, [d] Relative gap: 1.05%

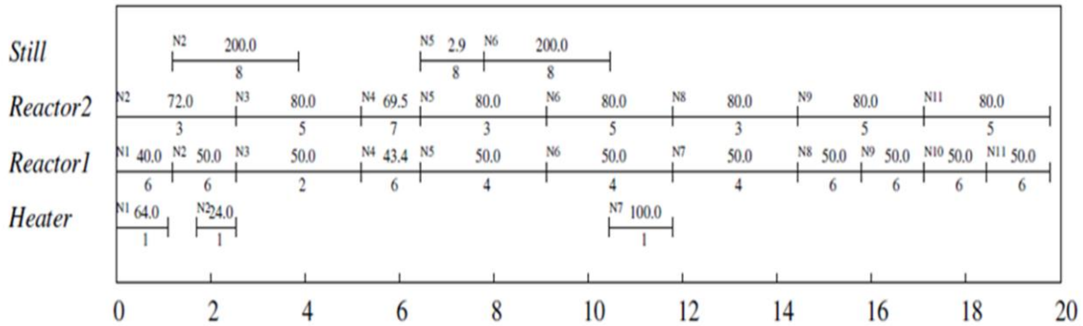


Fig. 4.3. Gantt chart for motivating example for cycle time range of 18 – 21h

4.3.2. Example 4.1

The example 4.1 is a simplified version of the motivating example and for the existing motivating example data, the following modifications are incorporated. (Schilling and Pantelides (1999)): (i) absence of heating process (ii) maximum possible storage capacity for hot A is 1000 mass units (mu) (iii) intermediate AB is produced only from reaction2 which takes place in reactor1 (iv) all the units have maximum possible capacity of 80 mu with different minimum capacities as 20 mu for reactor1, 30 mu for reactor2 and 40 mu for separator respectively (v) all tasks processing times are multiplied by 10 as compared to that of motivating example (vi) the product2 price is increased by 2 $/mu, therefore, the new selling price of 12 $/mu is considered.

Fig. 4.4 describes the process configuration using STN representation. The performance evaluation of the proposed mathematical formulation is determined based on predominant parameters like optimal objective value, cycle time and model statistics. The example 4.1 is solved for different cycle time ranges such as 20-40 h, 40-70 h up to 200-240 h and the results are listed in Table 4.4. Tabulated results imply that, for most of the problem instances the proposed model requires less number of event points in comparison to Wu and Ierapetritou (2004) model. For a cycle time range of 200-240 h both models resulted in the same objective value but better optimal cycle time is reported at higher Δn with the proposed model and the optimal Gantt chart is shown in Fig. 4.5. The tasks 7 and 3 are starting at event point 12 and ending at event point 1.

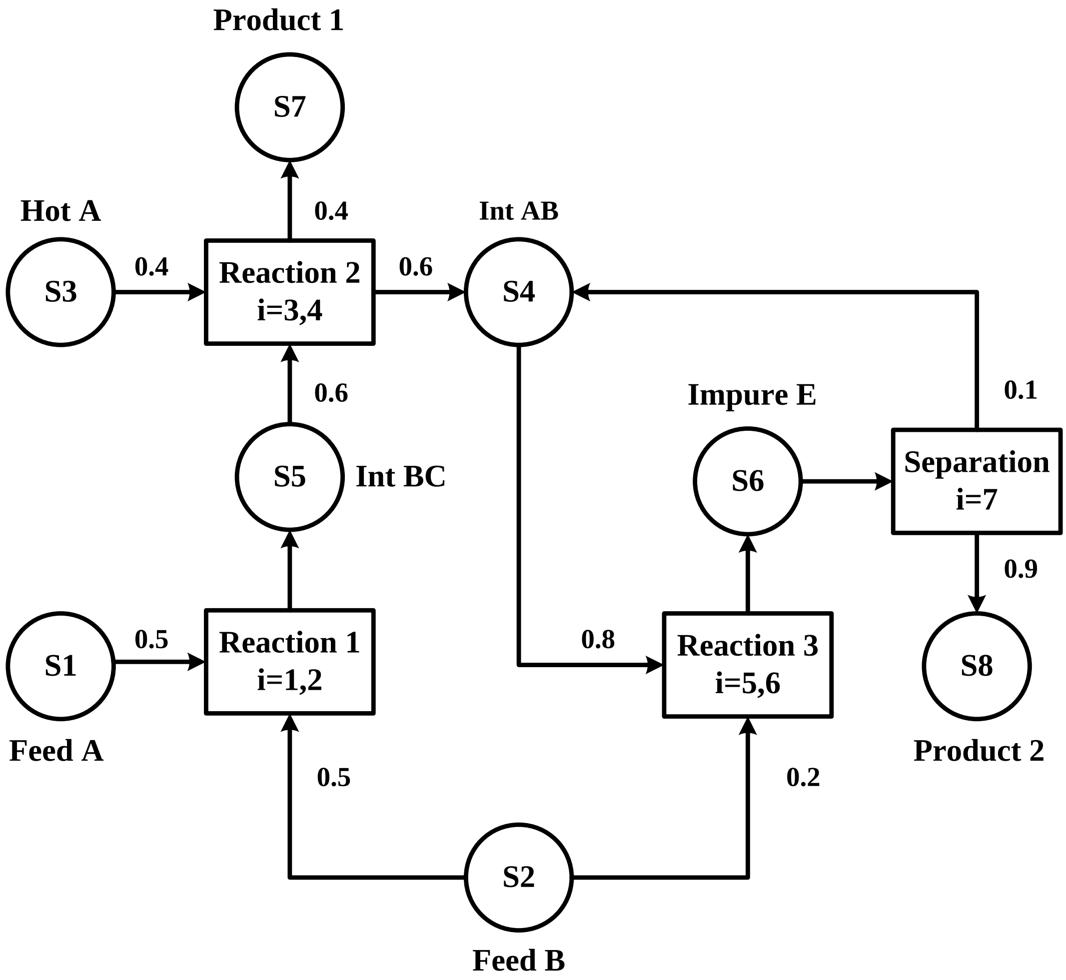


Fig. 4.4. STN representation for Example 4.1

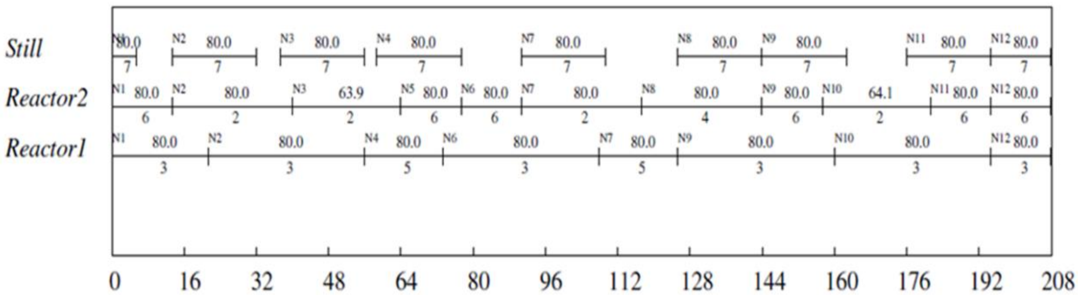


Fig. 4.5. Gantt chart for Example 4.1 for the range of 200-240h

4.3.3. Example 4.2

In this example, three raw materials are used for producing four final products. Eight tasks are involved in the process of converting raw materials into products. The STN representation of the process is shown in Fig. 4.6 and the required data is tabulated in Table 4.5.

Table 4.4. Computational results for Example 4.1

Model	Cycle time range (h)	Events	MINLP (Profit/h)	RMINLP (Profit/h)	Optimal cycle time (h)	CPU time (s)	Binary variables	Continuous variables	Constraints
Wu & Ierapetritou	20-40	3	28.942	--[a]	36.645	0.82	--[a]	--[a]	--[a]
This work	20-40	2	28.947	43.809	36.638	0.200	14	61	117
Wu & Ierapetritou	40-70	5	32.893	--[a]	62.540	25.78	--[a]	--[a]	--[a]
This work (Δn=1)	40-70	5	32.900	43.008	62.527	104.87	70	183	552
Wu & Ierapetritou	70-100	5	33.829	--[a]	93.333	10.00	--[a]	--[a]	--[a]
This work	70-100	4	33.840	37.113	93.310	1.400	28	119	267
Wu & Ierapetritou	100-140	6	34.321	--[a]	102.828	109.27	--[a]	--[a]	--[a]
This work	100-140	5	34.331	37.149	102.797	24.710	35	148	342
Wu & Ierapetritou	140-170	8	34.434	--[a]	159.048	5601.49	--[a]	--[a]	--[a]
This work	140-170	7	34.442	36.296	159.009	163.95	49	206	492
Wu & Ierapetritou	170-200	10	34.957	--[a]	171.575	312.67	--[a]	--[a]	--[a]
This work	170-200	11	34.968	38.062	171.522	10803.11	77	322	792
Wu & Ierapetritou	200-240	11	34.725	--[a]	223.240	6020.55	--[a]	--[a]	--[a]
This work (Δn=1)	200-240	12	34.777	36.384	207.952	20000[b,c]	168	435	1371

--[a] Not reported, [b]Resource limit reached, [c]Relative gap: 1.92%

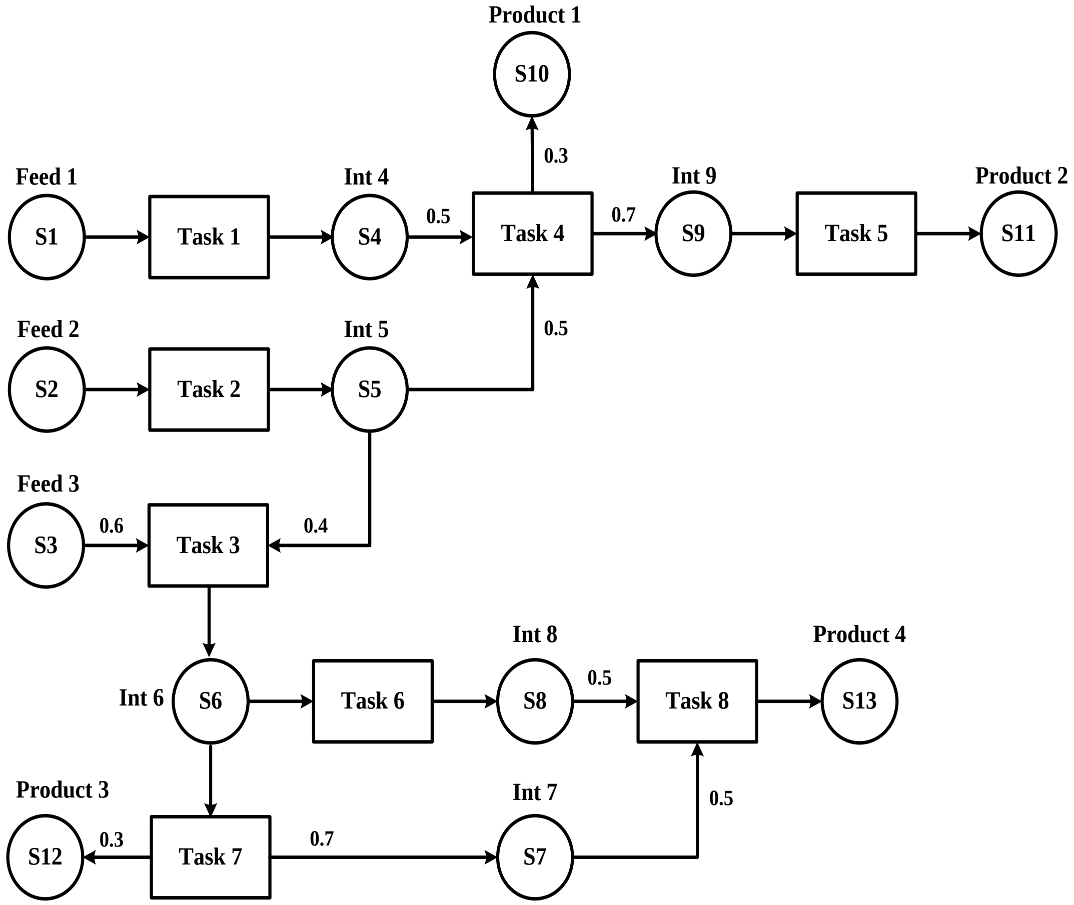


Fig. 4.6. STN representation for Example 4.2

Using the proposed mathematical formulation, this example is solved for different cycle time ranges such as 2-6, 6-9, up to 21-24 and computational results are reported in Table 4.6. The optimal Gantt chart for a cycle time range 9-12 h is shown in Fig. 4.7. Tabulated results of different problem instances elaborate that the proposed model consistently require less number of event points as compared with the Wu and Ierapetritou (2004) model.

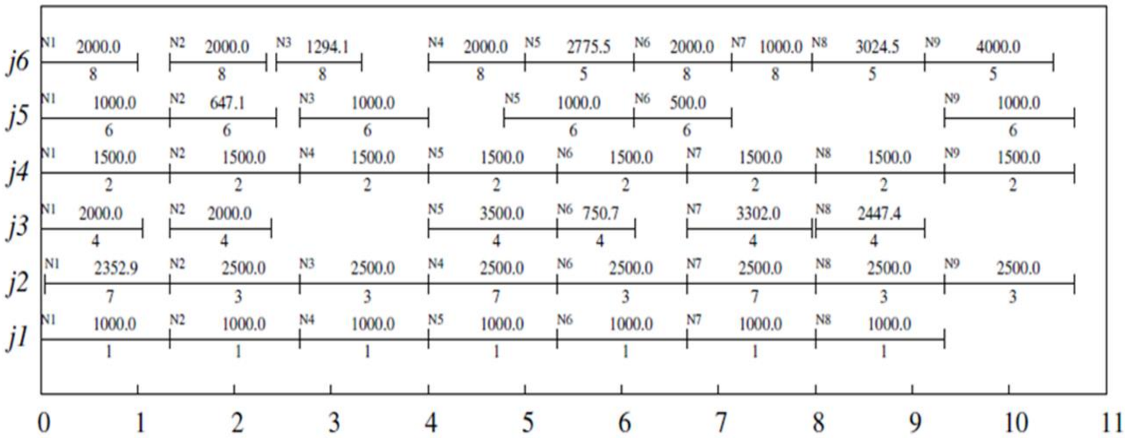


Fig. 4.7. Optimal Gantt chart for Example 4.2

Table 4.5. Data for Example 4.2

Unit(j)	Task(i)	Min. Batch size (mu)	Max.Batch size (mu)	Duration(h)
Unit (j1)	Task 1	0	1000	1
Unit (j4)	Task 2	0	1500	1
Unit (j2)	Task 3	0	2500	1
Unit (j3)	Task 4	0	3500	1
Unit (j6)	Task 5	0	4000	1
Unit (j5)	Task 6	0	1000	1
Unit (j2)	Task 7	0	1500	1
Unit (j6)	Task 8	0	4000	1
States	**Initial Amount (mu)**	**Storage capacity (mu)**	**Price ($/mu)**	
S1-S3	Unlimited	Unlimited	0	
S4	0	1000	0	
S5	0	1000	0	
S6	0	1500	0	
S7	0	2000	0	
S8	0	0	0	
S9	0	2000	0	
S10-S14	0	Unlimited	18-21	

4.3.4. Example 4.3: Cyclic scheduling with heat integrated mode

Generally, the scheduling problem instances with a longer time horizon lead to an increase in model size and difficult to obtain the optimal solution. Further, the addition of heat integration makes the solution of problems falls in the realm of high complexity. Cyclic scheduling creates the possibility of the reduction in complexity by diminishing the overall problem size by splitting up of overall time horizons into cycles of an equal time period. The unified model with heat integration constraints presented in section 3.2 is used to solve the example 3.2 from Chapter 3. The STN is shown in Fig. 3.4 and the corresponding scheduling data is given in Table 3.3.

In this process the final product S6 is produced through five processing stages: reaction1, reaction2, and reaction3, settling and evaporation. Materials S1 and S9 are conveyed into reactors R1 and R2 where reaction1 takes place and intermediate S2 is produced. The intermediate S2 along with raw material S10 are processed in reactors R3 and R4 where reaction2 takes place and intermediate S3 is produced. Further, the intermediate S3 along with raw material S11 are processed in reactors R3 and R4 where reaction3 takes place and intermediate S4 is produced. The intermediate S4 also known as monosodium salt solution is further processed through a series of settlers SE1, SE2, SE3, and solid byproduct S8 is removed. The remaining excess amount of water is removed by further processing it in a series of evaporators EV1 and EV2. The selling price of the final product S6 is 100 $/mu and the respective unit costs of cooling water are 8 $/mu and that of steam is 15 $/mu.

Table 4.6. Computational results for Example 4.2

Model	Cycle time range (h)	Events	MINLP (Profit/h)	RMINLP (Profit/h)	Optimal cycle time (h)	CPU time (s)	Binary variables	Continuous variables	Constraints
Wu & Ierapetritou	2-6	5	48305.00	--[a]	4.00	3.21	--[a]	--[a]	--[a]
This work	2-6	3	48309.831	57300.5	4.00	0.540	24	109	182
Wu & Ierapetritou	6-9	7	48671.471	--[a]	6.66	10.51	--[a]	--[a]	--[a]
This work	6-9	6	48676.338	53455.8	6.66	9.000	48	217	386
Wu & Ierapetritou	9-12	10	48946.324	--[a]	10.66	42.55	--[a]	--[a]	--[a]
This work	9-12	9	48951.219	52268.3	10.66	71.860	72	325	590
Wu & Ierapetritou	12-15	13	48871.364	--[a]	14.66	12271.43	--[a]	--[a]	--[a]
This work	12-15	12	48876.251	50880.2	14.66	157.430	96	433	794
Wu & Ierapetritou	15-18	15	48840.611	--[a]	17.33	3234.48	--[a]	--[a]	--[a]
This work	15-18	14	48845.495	50402.7	17.33	1387.700	112	505	930
Wu & Ierapetritou	18-21	16	48750.000	--[a]	18.66	1300.80	--[a]	--[a]	--[a]
This work	18-21	15	48754.875	49712.1	18.66	354.340	120	541	998
Wu & Ierapetritou	21-24	20	48946.324	--[a]	21.33	900.94	--[a]	--[a]	--[a]
This work	21-24	18	48951.219	49779.8	21.33	3407.34	144	649	1202

--[a] Not reported

In order to have a fair comparison with the Chen and Chang (2009) model, this example is solved for the objective of maximization of profit for fixed cycle time instances such as 2, 3, 4 up to 10 hours. Each of them is solved independently to find the maximum profit per hour. Similar to the Chen and Chang (2009) model the optimal cycle time is found to be 9h and the model requires 5 event points to get the optimal objective value of 161.08 profit/h. The optimal Gantt chart with highlighting the tasks scheduled in the heat integration mode is shown in Fig. 4.8. This clearly gives an idea and benefit of applying heat integration in cyclic scheduling. The computational results along with model statistics for all problem instances are presented in Table 4.7.

Further, the model is extended to find the optimal cyclic time from the specified range with an overall objective of profit maximization per hour. The prediction of the optimal cycle time is more complex and challenging as the model requires additional constraints and becomes non-linear in nature. Computational results for different cycle time ranges such as 3-9, 6-12, 9-15, and 12-18 are reported in Table 4.8. Tabulated results show that for a cycle time range 3-9, the maximum profit per hour is obtained at the cycle time of 7 hours and the Gantt chart is shown in Fig. 4.9. The same can be observed from Table 4.7 where cycle time is considered as a parameter. However, for the other cycle time ranges, new optimal solutions are witnessed at different cycle times as can be observed from Table 4.8. For the instance of the cycle time range of 12-18 h, the proposed model requires 9 events to obtain an objective value of 170.56 and cycle time of 17 h which require 135 binary variables, 543 continuous variables and 1506 number of equations. The optimal Gantt chart for a cycle time range of 12-18 h is shown in Fig. 4.10. Therefore, in the cyclic scheduling considering cycle time as a variable, better optimal solutions can be obtained as demonstrated in this case study.

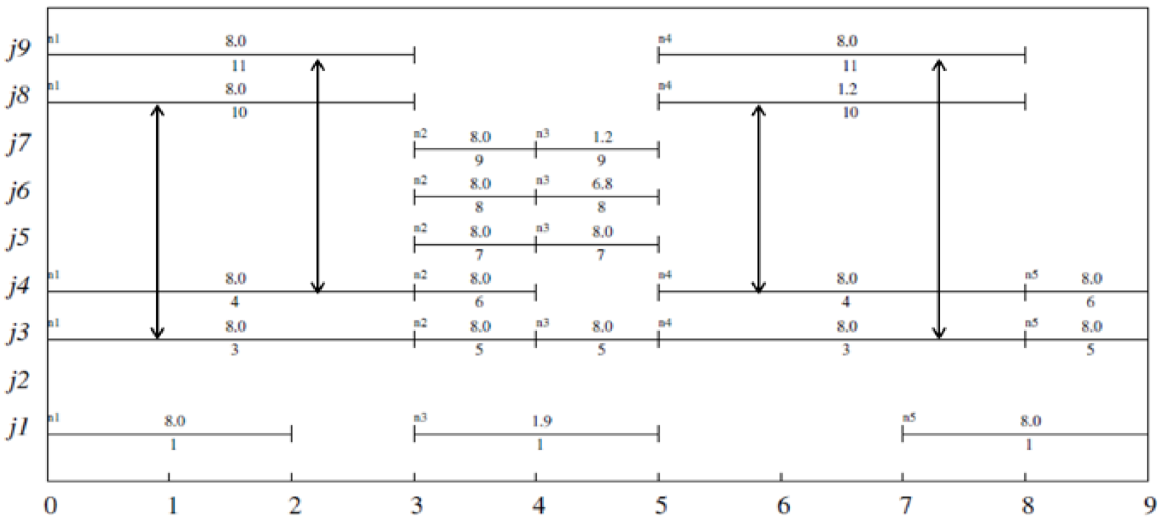


Fig. 4.8. Gantt chart for cyclic scheduling with heat integration for optimal cycle time 9h

Table 4.7. Computational results for the Example 4.3 at constant cycle time

H	Events	MILP	RMILP	Profit/h	CPU time	Binary variables	Continuous variables	Constraints
2	--[a]	--[a]	--[a]	--[a]	--[a]	--[a]	--[a]	--[a]
3	2	362.44	632.04	120.81	0.156	30	122	288
4	2	576.70	644.33	144.17	0.187	30	122	288
5	3	724.88	966.50	144.97	0.203	45	182	462
6	4	865.05	1288.67	144.17	0.328	60	242	636
7	4	1087.32	1288.67	155.33	0.390	60	242	636
8	4	1153.40	1288.67	144.17	0.172	60	242	636
9	5	1449.76	1610.84	161.08	0.250	75	302	810
10	5	1449.76	1610.84	144.97	0.265	75	302	810

--[a] Not Applicable

Table 4.8. Computational results for the Example 4.3 with cycle time as a variable

Cycle time range(h)	Number of events points	MINLP (Profit/h)	RMINLP	Optimal cycle time(h)	CPU time(s)	Binary variable	Continuous Variable	Constraints
3-9	4	155.331	359.084	7.000	5.890	60	243	636
6-12	7	164.745	308.745	11.000	46.970	105	363	1158
9-15	9	169.139	273.874	15.000	594.73	135	543	1506
12-18	9	170.560	241.627	17.000	259.67	135	543	1506

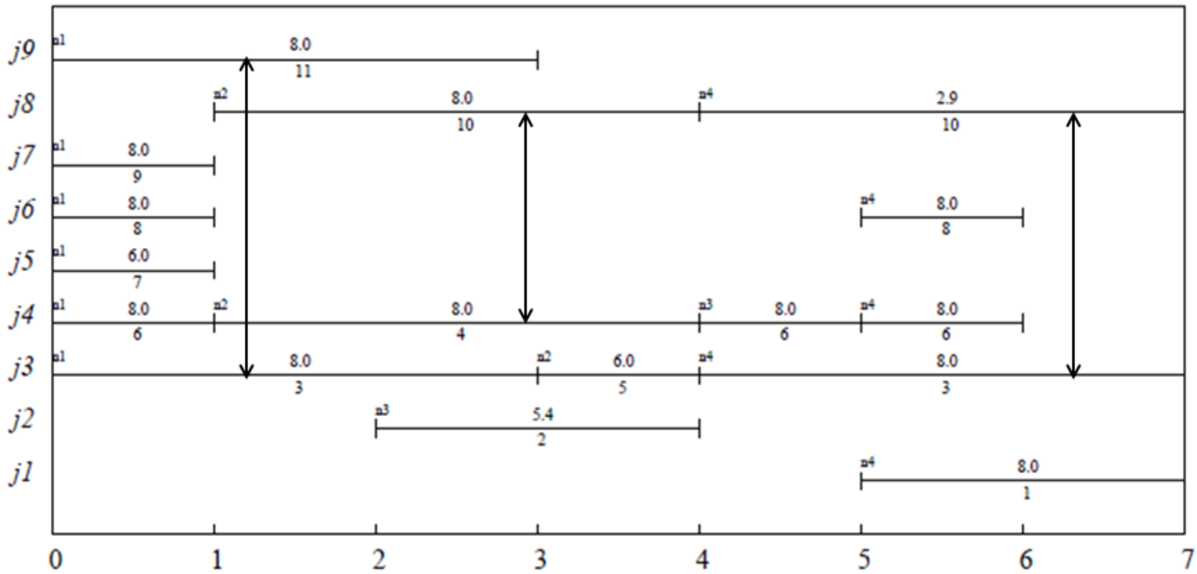


Fig. 4.9. Gantt chart for cyclic scheduling with heat integration for a cycle time range of 3-8 h

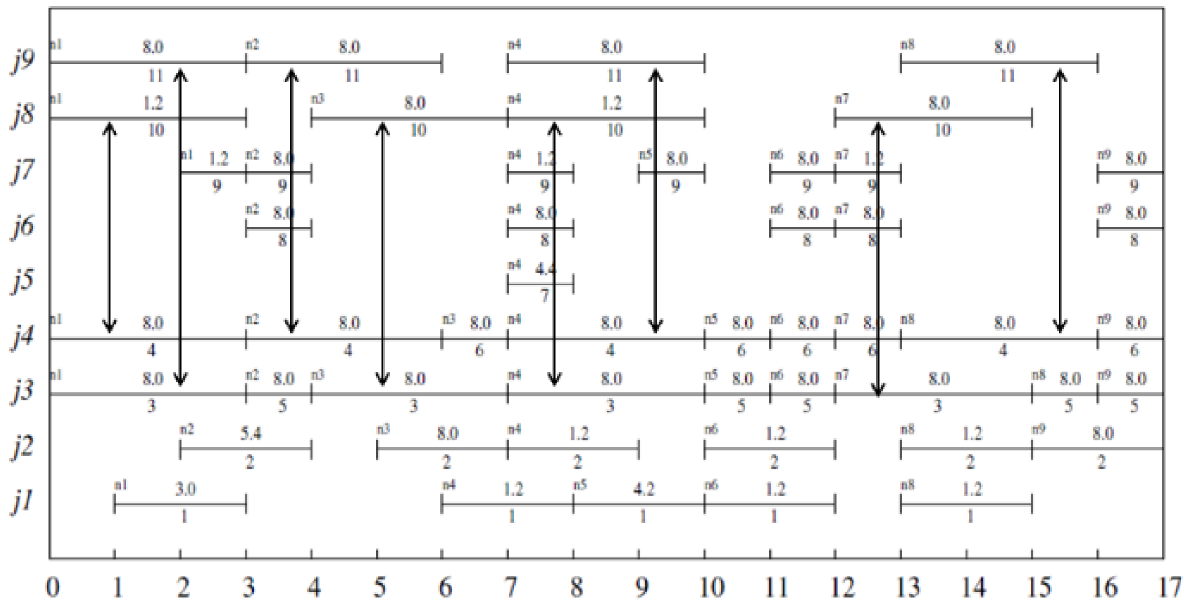


Fig. 4.10. Gantt chart for cyclic scheduling with heat integration for a cycle time range of 12-18h

4.4. Conclusions

In this work, a novel, continuous time three index unit-specific event-based model is proposed for cyclic scheduling of batch plants. The proposed unified framework will reduce to simple short term scheduling model in the absence of cyclic scheduling. Three examples from the literature are considered to evaluate the computational performance of the proposed unified framework. The computational results highlighted that the proposed formulation is superior in terms of model statistics than that of Wu and Ierapetritou (2004) model. This is due to the integration of active task concept in cyclic scheduling using three index binary and continuous variables. Further, the proposed framework can get better optimal results for three case studies of motivating example and one case study of example one. The unified framework is also extended to handle simultaneous scheduling and direct heat integration. The computational performance of the proposed model is evaluated by solving the industrial case study presented by Chen and Chang (2009). The computational results presented in Table 4.8 demonstrated that better optimal solutions could be obtained when the cycle time horizon is considered as a variable.

CHAPTER 5

UNIT SPECIFIC EVENT BASED MODEL FOR SHORT TERM SCHEDULING AND HEAT INTEGRATION OF BATCH PLANTS: DESIGN AND OPTIMIZATION OF HEAT STORAGE VESSELS

Unit specific event based model for short term scheduling and heat integration of batch plants: Design and optimization of heat storage vessels

Energy conservation has been one of the prime research objectives of the global scientific community to curb the CO2 emissions. Among unit operations used in the chemical industry, distillation, drying and evaporation are highly energy intensive. Process heat integration has been a promising intensification technique for energy conservation in the chemical industries. Further, the scope of heat integration has been expanding by including different scheduling aspects. Continuous-time modelling approach have evolved as a promising option for handling simultaneous scheduling and heat integration of batch plants. Among the different continuous-time modeling approaches available in the literature, unit specific event or slot based approach have evolved as better alternative as they generally require lesser number of events or slots to find optimal schedules compared to single-time grid models (synchronized slot-based and global-event based models).

To meet the objective 2.5.3 defined in chapter 2, a simple unit specific event based framework for batch plants is proposed for short term scheduling and heat integration along with design and optimization of storage vessels. Using the concept of active task and unit specific events, various modelling issues such as task alignments, energy balances, design of heat storage vessels, direct and indirect heat integrations have been handled precisely with a minimum number of equations and variables. The effect of the amount of thermal fluid, initial temperature and number of storage vessels on objective function is systematically analyzed. The accuracy and computational efficiency of the proposed framework is demonstrated using three benchmark examples taken from literature. The computational results highlight the necessity of direct heat integration for getting better optimal results in design and optimization of multiple heat storage vessels.

5.1. Problem statement

In this chapter, simultaneous scheduling and heat integration problem is formulated as two different cases. The first case mainly deals with the scheduling and heat integration with design and optimization of a single heat storage vessel. The amount of thermal fluid and initial temperature are the key decision variables considered for optimization. The scheduling problem needs data related to process and production recipe, duration of the task, size of equipment, equipment operational capacity, time horizon of interest, the cost of raw material and the selling price of products. Whereas, the heat integration problem can be specified using the following parameters: tasks that require heating and cooling, process heat loads, type of available utilities, costs of hot and cold utilities, duration of heat integrated tasks, task operating temperature, availability of heat storage vessels, temperature range of thermal fluid and minimum temperature approach. The overall objective is to maximize the total profit, which is represented as the difference between revenue from the product and cost associated with the utilities.

The second case deals with design and optimization of multiple heat storage vessels. In addition to the data specified for the first case, the following data is required to specify the problem: storage vessel data viz., capital cost, minimum and maximum capacity, heating and cooling tasks data viz., heat capacities, initial and final temperatures. The same objective function specified in the first case is evaluated for multiple storage vessels by incorporating their capital costs.

In both cases, the main objective is to optimize the use of direct and indirect heat integration in batch plants, as this is a scenario more often encountered in industrial applications. Towards this end, a unit specific event based (multiple time grid) framework is proposed for simultaneous scheduling and heat integration of batch plants with design and optimization of heat storage vessels. The final goal, as in case of all the other optimization problems, is to improve the net profit, considering the important industrial constraints.

These objective functions are sensitive to the following key decision variables and input parameters: minimum temperature approach, utility cost, batch processing amounts, number of available heat storage vessels, amount of thermal fluid and temperature. The following assumptions have been made: zero material transfer time, no unexpected unit failures, zero unit wait, no simultaneous heat exchange from the units, no heat loss from the units, heat exchanger capital cost is not considered in profit maximization and heat capacity is independent of temperature.

5.2. Mathematical formulation

The proposed formulation consists of simplified unit specific event based mathematical models, which can be used for scheduling and heat integration of batch plants with heat storage vessels. The proposed models can handle both direct and indirect heat integration by using a set of simple energy balance constraints. Using a novel 'unit specific event based modelling approach' and 'active task concept' a simple MINLP model is proposed which avoids the need of bilinear and trilinear terms for linearizing the indirect heat integration modelling aspects. The heat integration framework consists of allocation constraints, energy balance constraints, thermal fluid temperature constraints and heat exchange duration constraints. The scheduling constraints presented in chapter 3 are directly adopted in this chapter.

5.2.1. Heat integration model for design and optimization of single storage vessel

5.2.1.1. Allocation Constraints

Constraint (5.1) ensures that a processing task which requires heating can be integrated with a task requiring cooling. Alternatively, it can be integrated with heat exchange from a storage vessel. Similar integration can be achieved using Constraint (5.2) for a task which requires cooling. These two constraints ensure one to one mapping of heat source and sink while exchanging heat. In the absence of a match between the source and sink, the tasks can still be active by incorporating the required heat duty from the external utility.

$$\sum_{i' \in I_c} x(i,i',n) + \sum_{u} hex(i,u,n) \leq \sum_{\substack{n' \in N \\ n \leq n' \leq n+\Delta n}} w(i,n,n'),$$

$$\forall\ i \in I_h, i \neq i', n \in N \qquad (5.1)$$

$$\sum_{i \in I_h} x(i,i',n) + \sum_{u} hex(i',u,n) \leq \sum_{\substack{n' \in N \\ n \leq n' \leq n+\Delta n}} w(i',n,n'),$$

$$\forall\ i' \in I_c, i \neq i', n \in N \qquad (5.2)$$

Constraint (5.3) guarantees that at any event point, only one processing task can be integrated with the storage vessel for heat exchange.

$$\sum_{i \in I_h} hex(i,u,n) + \sum_{i' \in I_c} hex(i',u,n) \leq 1, \qquad \forall\ u \in U, n \in N \qquad (5.3)$$

Using three index binary variable $w(i,n,n')$, the direct and indirect heat integration alignments between heat source and sink are modelled with only three constraints. Whereas the SSN represented models require seven constraints to handle this task.

5.2.1.2. Energy Balance Constraints

Constraints (5.4) and (5.5) depict the energy balance of cooling and heating tasks. Constraint (5.4) states that the amount of cold utility required by cooling task i is satisfied from the following three possibilities: direct process heat integration, indirect heat integration using heat storage vessel and external utility. In case of direct or indirect heat integration, the deficit energy demand is compensated by using external utility. Similarly heating tasks requiring hot utility are taken care by Constraint (5.5).

$$qmt(i) \sum_{\substack{n' \in N \\ n \leq n' \leq n+\Delta n}} w(i,n,n') = q(i,n) + qs(i,u,n) +$$

$$\sum_{i' \in I_h} \Big(x(i',i,n) min\big(qmt(i), qmt(i')\big)\Big), \qquad \forall\ i \in I_c, u \in U, n \in N \qquad (5.4)$$

$$qmt(i) \sum_{\substack{n' \in N \\ n \leq n' \leq n+\Delta n}} w(i,n,n') = q(i,n) + qs(i,u,n) +$$

$$\sum_{i' \in I_c} \Big(x(i,i',n) min\big(qmt(i), qmt(i')\big)\Big), \qquad \forall\ i \in I_h, u \in U, n \in N \qquad (5.5)$$

Constraints (5.6) and (5.7) ensure that the finishing time of heating and cooling tasks are equal when they are in direct heat integration at event point *n*. The heating task *i* which is active from event *n* to *n1* is aligned with cooling task *i'* active from event *n* to *n1*. This ensures that the heating and cooling tasks are active at the same time interval on a real time horizon.

$$T^f(i,n') \geq T^f(i',n1) - M\big(3 - x(i,i',n) - w(i,n,n') - w(i',n,n1)\big),$$
$$\forall\ i \in I_h, i' \in I_c, n, n', n1 \in N, n \leq n' \ \leq n + \Delta n, n \leq n1 \leq n + \Delta n \tag{5.6}$$

$$T^f(i,n') \leq T^f(i',n1) + M\big(3 - x(i,i',n) - w(i,n,n') - w(i',n,n1)\big),$$
$$\forall\ i \in I_h, i' \in I_c, n, n', n1 \in N, n \leq n' \ \leq n + \Delta n, n \leq n1 \leq n + \Delta n \tag{5.7}$$

Constraints (5.8) and (5.9) calculate the amount of energy transferred from the thermal fluid to processing tasks, which require heating. Constraints (5.10) and (5.11) allow energy transfer from heat storage vessel to processing task only when they are integrated. Similarly, constraints (5.12) to (5.15) ensure energy transfer from processing task to heat storage vessel when they are integrated. Constraints (5.8), (5.9), (5.12) and (5.13) also decide the final temperature of the thermal fluid based on the amount of heat exchanged. These energy balance constraints are formulated as second order non-linear equations using three index binary and continuous variables. In SSN formulations, third order non-linear energy balance equations were used to model the indirect heat integration.

$$qs(i,u,n) \geq wt(u)C_p(u)\left(TT^s(u,n) - TT^f(u,n)\right) - MM\big(1 - hex(i,u,n)\big),$$
$$\forall\ i \in I_h, u \in U, n \in N \tag{5.8}$$

$$qs(i,u,n) \leq wt(u)C_p(u)\left(TT^s(u,n) - TT^f(u,n)\right) + MM\big(1 - hex(i,u,n)\big),$$
$$\forall\ i \in I_h, u \in U, n \in N \tag{5.9}$$

$$qs(i,u,n) \geq 0.0001hex(i,u,n), \qquad \forall\ i \in I_h, u \in U, n \in N \tag{5.10}$$

$$qs(i,u,n) \leq MM\ hex(i,u,n), \qquad \forall\ i \in I_h, u \in U, n \in N \tag{5.11}$$

$$qs(i,u,n) \geq wt(u)C_p(u)\left(TT^f(u,n) - TT^s(u,n)\right) - MM\big(1 - hex(i,u,n)\big),$$
$$\forall\ i \in I_c, u \in U, n \in N \tag{5.12}$$

$$qs(i,u,n) \leq wt(u)C_p(u)\left(TT^f(u,n) - TT^s(u,n)\right) + MM\big(1 - hex(i,u,n)\big),$$
$$\forall\ i \in I_c, u \in U, n \in N \tag{5.13}$$

$$qs(i,u,n) \geq 0.0001hex(i,u,n), \qquad \forall\ i \in I_c, u \in U, n \in N \tag{5.14}$$

$$qs(i,u,n) \leq MM\ hex(i,u,n), \qquad \forall\ i \in I_c, u \in U, n \in N \tag{5.15}$$

Constraint (5.16) states that the initial temperature of thermal fluid at an event point *n* is equal to final temperature at an event point *n*-1. In the absence of energy exchange, the thermal fluid initial and final temperatures at event point *n* are equal as shown in Constraints (5.17) and (5.18). Using Constraints (5.19) and (5.20) the minimum temperature approach ΔT_{min} is ensured between the hot and cold streams during heat exchange. Constraint (5.21) ensures the thermal fluid temperature is within the specified maximum and minimum limits.

$$TT^s(u,n) = TT^f(u,n-1), \qquad \forall\ u \in U, n \in N, n > 1 \tag{5.16}$$

$$TT^s(u,n) \le TT^f(u,n) + T^u(u)\left(\sum_{i \in I_h} hex(i,u,n) + \sum_{i' \in I_c} hex(i',u,n)\right),$$
$$\forall\ u \in U, n \in N \tag{5.17}$$

$$TT^s(u,n) \ge TT^f(u,n) - T^u(u)\left(\sum_{i \in I_h} hex(i,u,n) + \sum_{i' \in I_c} hex(i',u,n)\right),$$
$$\forall\ u \in U, n \in N \tag{5.18}$$

$$T_J(i) - TT^f(u,n) \ge \Delta T_{Min} - T^u(u)\big(1 - hex(i,u,n)\big),$$
$$\forall\ i \in I_c, u \in U, n \in N \tag{5.19}$$

$$TT^f(u,n) - T_J(i) \ge \Delta T_{Min} - T^u(u)\big(1 - hex(i,u,n)\big),$$
$$\forall\ i \in I_h, u \in U, n \in N \tag{5.20}$$

$$T^l(u) \ge TT^f(u,n) \ge T^u(u);\ \ T^l(u) \ge TT^s(u,n) \ge T^u(u),\ \ \forall\ u \in U, n \in N \tag{5.21}$$

Constraints (5.22) to (5.27) ensure the alignment of heat storage vessels with processing tasks when they are integrated at an event point *n*. Constraints (5.22) and (5.23) state that at event point *n* the starting time of heat exchange between the storage vessel and processing task are the same, when they are integrated. Similarly, Constraints (5.24) and (5.25) align the finishing times. The starting time of heat exchange in storage vessel *u* at event point *n* is always greater than the finishing time at previous event *n*-1 as shown in Constraint (5.26). Constraint (5.27) states that finishing time of heat exchange in storage vessel *u* is always greater than or equal to the starting time. Using the advantage of unit specific event alignments, the starting and finishing times of heat exchange between storage unit and processing task are modelled with minimum number of equations. These generic constraints will handle the batch processes with constant and variable process timings.

$$HT^s(u,n) \ge T^s(i,n) - M\big(1 - hex(i,u,n)\big), \qquad \forall\ i \in (I_c \cup I_h), u \in U, n \in N \tag{5.22}$$

$$HT^s(u,n) \le T^s(i,n) + M\big(1 - hex(i,u,n)\big), \qquad \forall\ i \in (I_c \cup I_h), u \in U, n \in N \tag{5.23}$$

$$HT^f(u,n) \ge T^f(i,n') - M\big(2 - hex(i,u,n) - w(i,n,n')\big),$$
$$\forall\ i \in (I_c \cup I_h), u \in U, n, n' \in N, n \le n' \le n + \Delta n \tag{5.24}$$

$$HT^f(u,n) \le T^f(i,n') + M\big(2 - hex(i,u,n) - w(i,n,n')\big),$$
$$\forall\ i \in (I_c \cup I_h), u \in U, n, n' \in N, n \le n' \le n + \Delta n \tag{5.25}$$

$$HT^s(u,n) \ge HT^f(u,n-1),\ \ \forall\ u \in U, n \in N, n > 1 \tag{5.26}$$

$$HT^f(u,n) \ge HT^s(u,n), \qquad \forall\ u \in U, n \in N \tag{5.27}$$

5.2.1.3. Objective function

Equation (5.28) depicts the objective function of the proposed problem. The variable Z represents the net profit, which is calculated as the difference between the revenue from the product and cost associated with the hot and cold utilities.

Maximize:

$$Z = \sum_{s \in S^p} price(s) \left(ST(S,N) + \sum_{i \in I_s^p} \rho_{is} \sum_{\substack{n' \in N \\ n-\Delta n \leq n' \leq n}} b(i,n',n) \right) - \sum_{i \in I_h} \sum_{n=1}^{N} \left(c_h q(i,n) \right) - \sum_{i' \in I_c} \sum_{n=1}^{N} \left(c_c q(i',n) \right) \quad (5.28)$$

The proposed heat integrated model equations from (5.1) to (5.28) and process scheduling model equations from (3.1) to (3.13) are used to solve the problem specified in the first case. The resulting MINLP model is iteratively solved by varying N and Δn until the objective function is converged. In the design and optimization of storage vessel, the constraints (5.8) and (5.9) become non-linear because the amount of thermal fluid and temperatures in enthalpy term are variables.

5.2.2. Heat integration model for design and optimization of multiple heat storage vessels

In this section, the model equations related to design of multiple heat storage vessels are presented. The equations 5.1, 5.2, 5.3, 5.6, 5.7, 5.8, 5.15 to 5.18 and 5.22 to 5.27 presented in Section 5.2.1 are directly used in this model along with the scheduling constraints (3.1) to (3.13) from Chapter 3. In addition to the above equations, a new set of modelling equations are presented in this section to handle the design of multiple heat storage vessels. The expression used for calculating the capital cost of the heat storage vessels are adopted from Sebelebele and Majozi (2017).

5.2.2.1. Capacity constraints

The constraints (5.29) and (5.30) enforce the size of heat storage vessel will be within the maximum and minimum capacity.

$$wt(u) \geq W^l(u) ns(u), \quad \forall\ u \in U, n \in N \quad (5.29)$$

$$wt(u) \leq W^u(u) ns(u), \quad \forall\ u \in U, n \in N \quad (5.30)$$

5.2.2.2. Heat storage vessel selection constraints

The heat storage vessel must be utilized at least once for heat exchange, if it exists in the process. In Equations (5.31) and (5.32), the binary variable *ns(u)* value of one represents the existence of heat storage vessel *u* in the process schedule. These constraints find the optimal number of heat storage vessels needed for indirect heat exchange at optimal objective value.

These constraints eliminate the iterative method used for estimating the optimal number of heat storage vessels required for heat exchange.

$$\sum_{\substack{i \in I_c \cup I_h \\ n \in N}} hex(i,u,n) \leq MM\, ns(u), \qquad \forall\ u \in U \tag{5.31}$$

$$\sum_{\substack{i \in I_c \cup I_h \\ n \in N}} hex(i,u,n) \geq ns(u), \qquad \forall\ u \in U \tag{5.32}$$

5.2.2.3. Energy balance constraints

Equations (5.33) and (5.34) calculate the energy loads of processing task *i*. These constraints handle the variable energy loads, which mainly depend on batch processing amount.

$$vqmt(i,n) = C_p(i)\left(T^{po}(i) - T^{pi}(i)\right) \sum_{\substack{n' \in N \\ n \leq n' \leq n+\Delta n}} b(i,n,n'),$$

$$\forall\ i \in I_h, n \in N \tag{5.33}$$

$$vqmt(i,n) = C_p(i)\left(T^{pi}(i) - T^{po}(i)\right) \sum_{\substack{n' \in N \\ n \leq n' \leq n+\Delta n}} b(i,n,n'),$$

$$\forall\ i \in I_c, n \in N \tag{5.34}$$

Constraints (5.35) and (5.36) ensure that the cooling or heating load required by task *i* is supplied from external utility, thermal fluid or other processing task. In the case of direct heat exchange scenario, the amount of heat exchange between two processing tasks is less than or equal to the minimum of the two energy loads as highlighted in Equation (5.37).

$$vqmt(i,n) = q(i,n) + \sum_{u \in U} qs(i,u,n) + \sum_{ii \in I_h} mqmt(ii,i,n),$$

$$\forall\ i \in I_c, n \in N \tag{5.35}$$

$$vqmt(i,n) = q(i,n) + \sum_{u \in U} qs(i,u,n) + \sum_{ii \in I_c} mqmt(i,ii,n),$$

$$\forall\ i \in I_h, n \in N \tag{5.36}$$

$$mqmt(i,ii,n) \leq x(i,ii,n) min\Big(C_p(i) B_i^{max}\left(T^{po}(i) - T^{pi}(i)\right),$$

$$C_p(ii) B_{ii}^{max}\left(T^{pi}(i) - T^{po}(i)\right)\Big), \qquad \forall\ i \in I_h, ii \in I_c, n \in N \tag{5.37}$$

The temperature approach between the processing task and thermal fluid should be greater than or equal to ΔT_{min}. Constraints (5.38) to (5.41) ensure specified ΔT_{min} between thermal fluid and processing task *i* at event *n* only when they are integrated.

$$T^{pi}(i) - TT^f(u,n) \geq \Delta T_{Min} - T^u(u)\left(1 - hex(i,u,n)\right),$$

$$\forall\ i \in I_c, u \in U, n \in N \tag{5.38}$$

$$T^{po}(i) - TT^s(u,n) \geq \Delta T_{Min} - T^u(u)\left(1 - hex(i,u,n)\right),$$

$$\forall\ i \in I_c, u \in U, n \in N \tag{5.39}$$

$TT^f(u,n) - T^{pi}(i) \geq \Delta T_{Min} - T^u(u)\big(1 - hex(i,u,n)\big),$

$\forall\ i \in I_h, u \in U, n \in N$ (5.40)

$TT^s(u,n) - T^{po}(i) \geq \Delta T_{Min} - T^u(u)\big(1 - hex(i,u,n)\big),$

$\forall\ i \in I_h, u \in U, n \in N$ (5.41)

5.2.2.4. Objective function

Equation (5.42) depicts the objective function of the proposed problem. The variable Z represents the net profit, which is calculated as the difference between the revenue from the product, annualized capital cost of the heat storage vessels and the cost associated with the hot and cold utilities.

Maximize:

$$Z = \left(\sum_{s \in S^p} price(s) \left(ST(S,N) + \sum_{i \in I_s^p} \rho_{is} \sum_{\substack{n' \in N \\ n-\Delta n \leq n' \leq n}} b(i,n',n) \right) - \sum_{i \in I_h} \sum_{n=1}^{N} \big(c_h q(i,n)\big) - \sum_{i' \in I_c} \sum_{n=1}^{N} \big(c_c q(i',n)\big) \right) \frac{hr/yr}{H} - \sum_{u \in U} \big(C_{cost} + V_{cost} wt(u)^{\theta}\big) ns(u)\, A_f \quad (5.42)$$

5.3. Important enhancements of the proposed framework

In the present work, the main objective is to optimize the use of direct and indirect heat integration in batch plants, as this is a scenario more often encountered in industrial applications. The STN represented unit specific event based models are proved to be computationally efficient for addressing wide variety of scheduling problems. For the first time, this modelling approach is explored to solve the simultaneous scheduling and heat integration (direct and indirect) of batch plants. The STN representation is used to characterize process flow sheet data.

A generic MINLP unit specific event based framework is proposed to handle simultaneous scheduling and heat integration of batch plants with design and optimization of multiple storage vessels. The final goal, as in case of all the other optimization problems, is to improve the net profit, considering the important industrial constraints. The alignment of direct and indirect heat integrated tasks is precisely modelled using active task concept. The value of three index binary variable $w(i,n,n')$ is used for deciding the direct or indirect heat integration possibilities of task i at event n. With this approach the number of constraints used for aligning the heat integration tasks at an event point n have been brought down to three, compared to seven of Stamp and Majozi (2011). A novel energy balance (Constraint 5.4 or 5.5) effectively handles the direct and indirect heat integration of task i. This energy balance constraint facilitates the partial utilization of external utilities to meet the energy deficiency for both direct and indirect heat integration.

This formulation eliminated the use of bilinear and trilinear terms for calculating the enthalpy of thermal fluid at an event point *n*. A set of second order non-linear equations with three index binary and continuous variables are formulated to handle the indirect heat integration. Unlike the Stamp and Majozi (2011) model, the proposed formulation does not require any decomposition methods to solve the simultaneous scheduling and heat integration problems with design of heat storage vessel. A set of generic duration constraints are proposed for aligning the starting and finishing times of heat source and sink. The same set of constraints takes care of alignment of batch processes with constant and variable processing times. This formulation does not ignore the direct heat integration possibilities while designing the multiple storage vessels. Further, the proposed formulation effectively handles the design and optimization of multiple storage vessels by finding the optimal number of storage vessels and calculating their sizes and initial temperatures.

5.4. Computational results

In the present work, three different examples from literature have been selected and investigated to demonstrate the computational effectiveness and accuracy of the proposed formulation. Examples 1 and 2, adopted from Stamp and Majozi (2011), deal with the design and optimization of a single storage vessel, whereas, Example 3 address the design and optimization of multiple heat storage vessels (Sebelebele and Majozi (2017)). The optimization solvers GAMS 24.4.1- CEPLEX and BARON are used to solve the linear and non-linear models respectively. The desktop computer consisting of Intel Xeon E5-1607 3.00 GHz processor with 8 GB RAM and Windows 7 operating system is used as a computational resource.

5.4.1. Example 5.1

The scheduling aspects of this example were first discussed by Sundaramoorthy and Karimi (2005). Stamp and Majozi (2011) modified this example by including heat integration possibilities. Fig. 5.1 shows the process recipe in the form of STN representation. The scheduling and heat integration data is given in Tables 5.1, 5.2 and 5.3. Three different operational scenarios have been evaluated: a) without heat integration b) direct heat integration and c) direct and indirect heat integration. The first two operational scenarios were solved by using the MILP direct heat integration model resulting from the proposed formulation and Stamp and Majozi (2011) model presented in Appendix (A). The third operational scenario was solved using MINLP solver by retaining the nonlinearity encountered in both models, while calculating initial and final enthalpies of the thermal fluid at each event. The computational results for these three scenarios are presented in Table 5.4. The operational scenario with direct and indirect heat integration has minimum utility requirements and hence resulted in maximum net profit as compared to the other two scenarios. The Gantt chart for this scenario using the proposed model is shown in Fig. 5.2. In the Gantt chart, the x-axis represent real time horizon in hours and y-axis represent processing units and heat storage vessels. The processing tasks are highlighted by using three identifiers including task number at the bottom, batch processing amount at the top and event number on the left side. The processing task in the Gantt chart can be read with the help of these three identifiers. For instance, in Fig. 5.2 at event *n*2 the task four is active in unit J3 (Reactor 2) and it is processing 120 mass units (mu) of material in the duration of 2 hours. Similarly, the heat storage vessel temperature changes along the real time horizon are also represented at different event points. The proposed formulation and Stamp and Majozi (2011) model resulted in the same optimal value for all three operational scenarios. However, for the first two problem instances, the proposed model required one less event as compared to Stamp and Majozi (2011) model. The proposed model consistently require less number of equations, binary and continuous variables than the Stamp and Majozi (2011) model. Subsequently, both the models resulted different optimal thermal fluid conditions for the direct and indirect heat integration scenario. This conclusion motivated us to further investigate the effect of thermal fluid amount and initial temperature on objective function.

Table 5.1. Scheduling data for the Example 5.1

Task(i)	**Unit(j)**	**Batch size (ton)**	**Processing time**	**States**	**Storage capacity (ton)**	**Initial Amount (ton)**	**Price (cu/ton)**
Heating1	Heater	100	1	S1	Unlimited	Unlimited	0
Heating2	Heater	100	1.5	S2	Unlimited	Unlimited	0
Reaction1	Reactor1	100	2	S3	100	0	0
Reaction1	Reactor2	150	2	S4	100	0	0
Reaction2	Reactor1	100	1	S5	300	0	0
Reaction2	Reactor2	150	1	S6	150	50	0
Reaction3	Reactor1	100	2	S7	150	50	0
Reaction3	Reactor2	150	2	S8	Unlimited	Unlimited	0
Separation	Separator	300	3	S9	150	0	0
Mixing	Mixer 1	200	2	S10	150	0	0
Mixing	Mixer 2	200	2	S11	Unlimited	Unlimited	0
				S12	Unlimited	0	5
				S13	Unlimited	0	5

Table 5.2. Heating/Cooling requirements for the Example 5.1

Task(i)	**Type**	**Operating temperature (^oC)**	**Heating/Cooling requirement (kWh)**
Reaction1	Exothermic	100	60 (cooling)
Reaction2	Endothermic	60	80 (heating)
Reaction3	Exothermic	140	70 (cooling)

Table 5.3. Heat integration data for the Example 5.1

Parameter	**Value**
Cooling water cost (cu/Kwh)	2
Steam cost(cu/Kwh)	10
Product selling price (cu/ton)	1,000
Specific heat capacity, c_p (kJ/kg^{o}C)	4.2
Lower bound for heat storage capacity (ton)	1
Upper bound for heat storage capacity (ton)	3
Minimum temperature difference, ΔT_{min} (^{o}C)	10
Lower bound for heat storage temperature (^{o}C)	20
Upper bound for heat storage temperature (^{o}C)	180

By considering the amount of thermal fluid as a parameter the nonlinearity in enthalpy term is eliminated. Further, the resulting MILP model is evaluated at different values of this parameter using the iterative procedure presented in Fig. 5.3. The effect of the amount of thermal fluid on the initial temperature of the storage vessel and net profit is presented in Fig. 5.4. It can be observed from the results that the heat exchange capacity of the vessel increases with increase in the amount of thermal fluid. Therefore, better heat exchange possibilities can be observed, which ultimately result in the maximum overall profit. For this example the maximum net profit of 224000 cu has been observed at 1.905 ton of thermal fluid and initial temperature of 82.5 ^{o}C. At these conditions the combined heat load of all processing tasks is met. Hence, further increase in the quantity of thermal fluid beyond 1.905 ton is superfluous. Net profit remains constant above 1.905 ton of thermal fluid.

As the amount of thermal fluid varies, the initial temperature is adjusted accordingly to satisfy the enthalpy balance and minimum temperature approach. From Fig. 5.5 it can be observed that the initial temperature of thermal fluid decreases as the amount increases, so that the ΔT_{min} = 10 ^{o}C is maintained at 4 hours where the pinch point exist for all the amounts of thermal fluid.

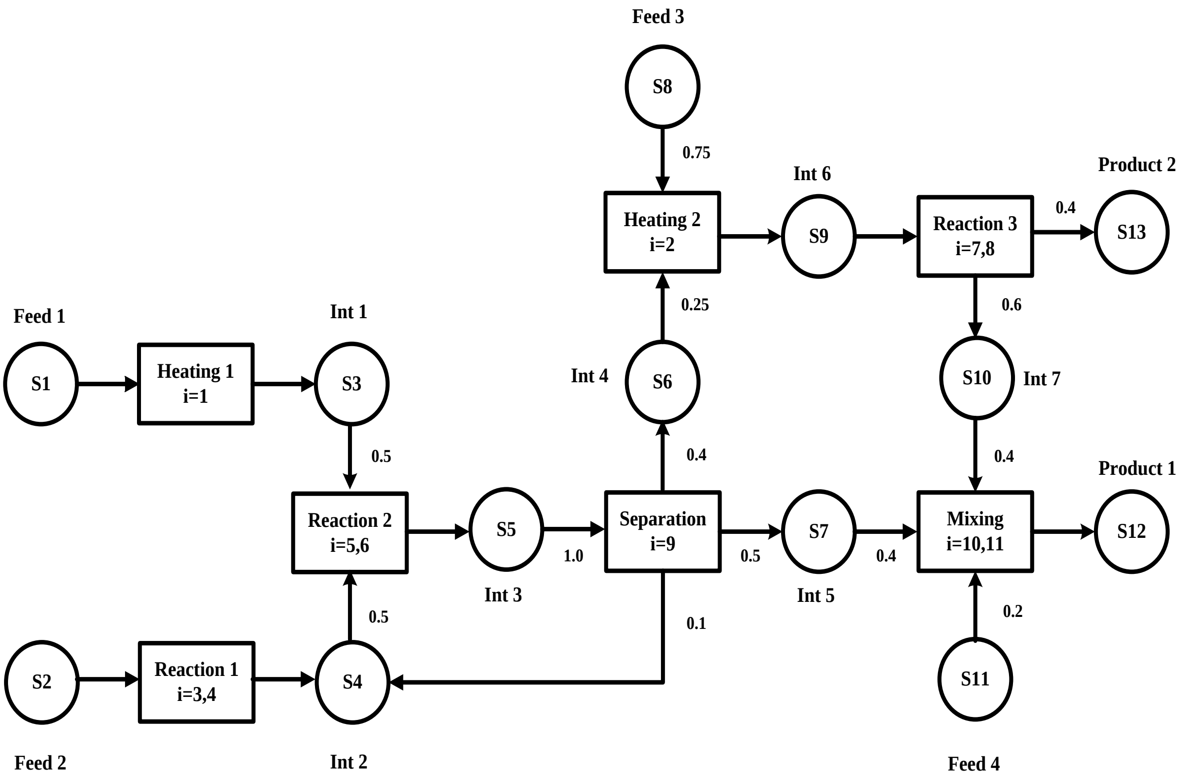


Fig. 5.1. STN representation for Example 5.1

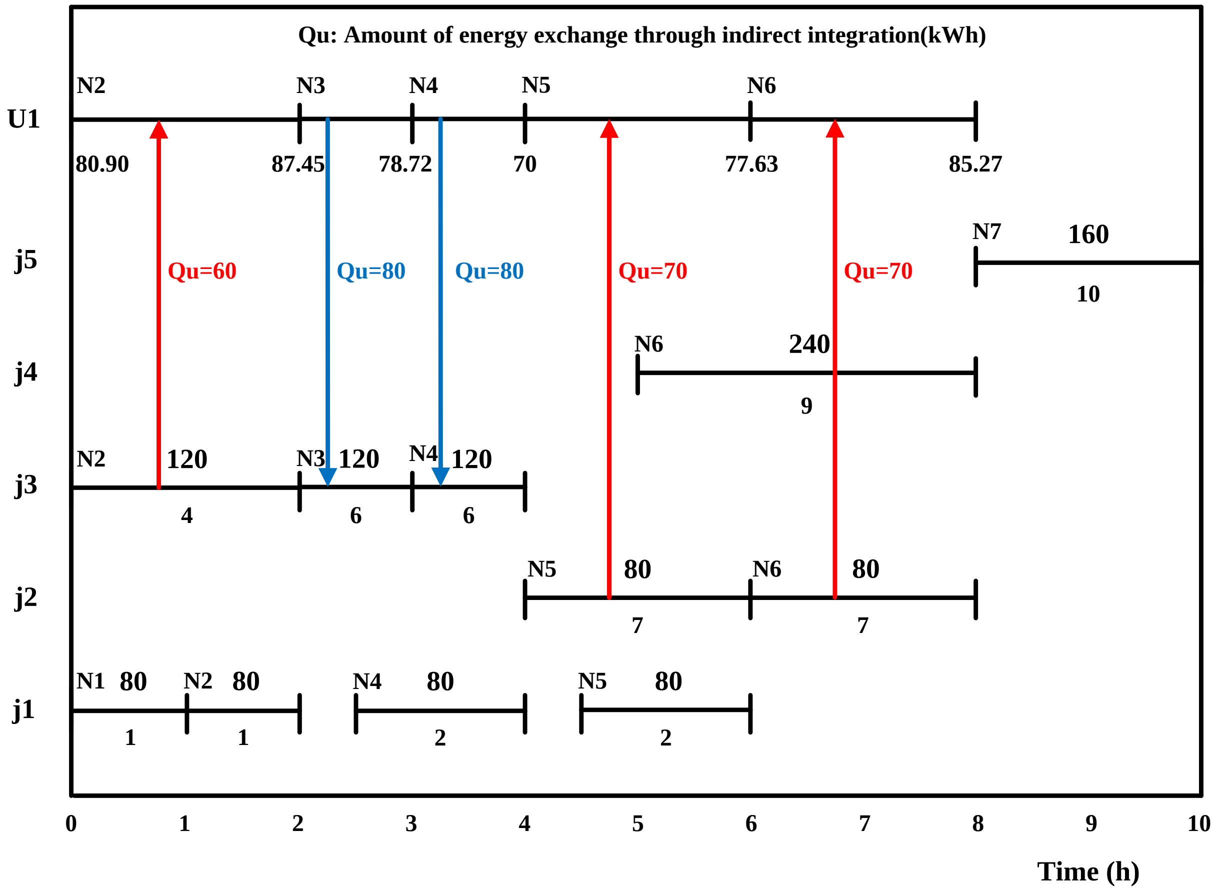


Fig. 5.2. Gantt chart for Example 5.1 with direct and indirect heat integration

```
Parameter i=1;
For (n=W^l(u) to W^u(u) by 0.05)
{
Solve resulting MILP problem for maximization of Z;
Oarray (i) = Z;
Marray (i) = n
i++;
}
Plot Oarray (i) vs Marray (i);
```

Fig. 5.3. Algorithm for calculating the optimal amount of thermal fluid

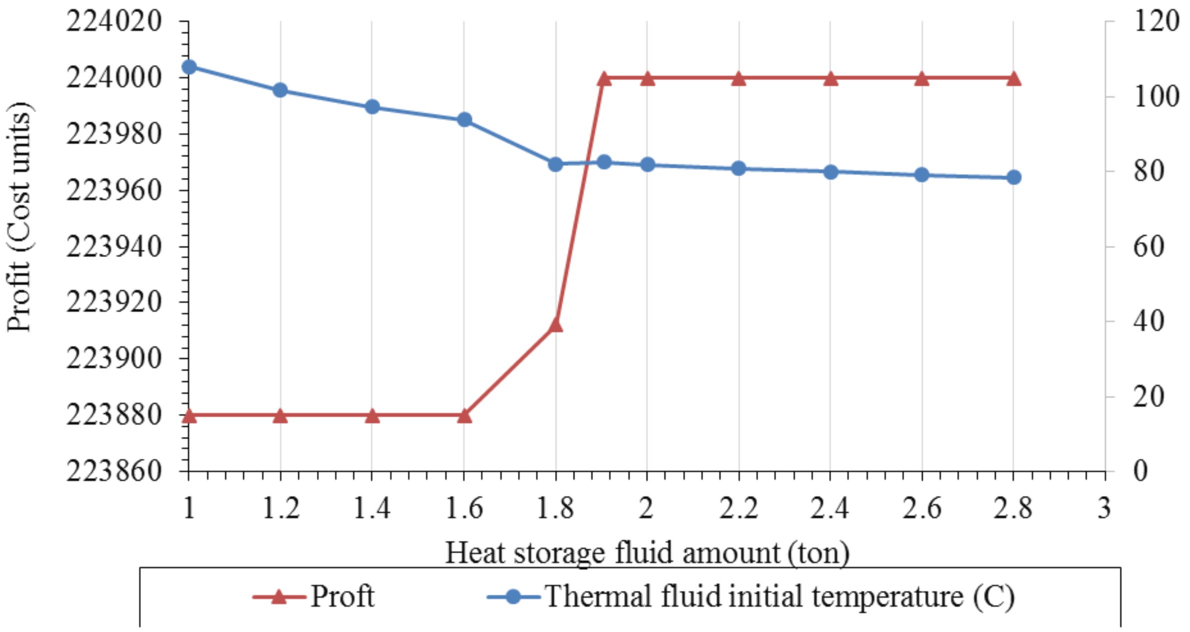


Fig. 5.4. Effect of amount of thermal fluid on net profit and initial temperature

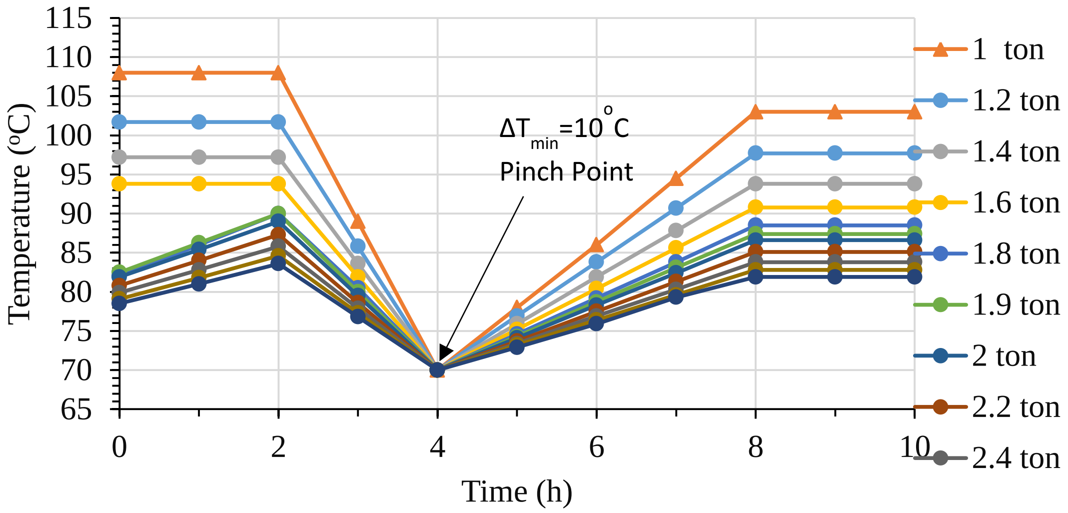


Fig. 5.5. Time dependent temperature profile for different amounts of thermal fluid

Table 5.4. Computational results for Example 5.1 and 5.2

Model	Events	Profit (c.u.)	External Hot Utility (kWh)	External Cold Utility (kWh)	Amount of Thermal Fluid (ton), Initial temperature (^{o} C)	CPU time (s)	Binary variables	Continuous Variables	Constraints
Example 5.1 - Without heat integration									
This work	6	222000	160	200		0.2	41	315	759
Stamp and Majozi (2011)	6	63720	0	140		0.04	66	472	995
	7	222000	160	200		0.2	77	553	1168
Example 5.1 – Direct heat integration									
This work	6	222840	90	130		0.2	89	351	927
Stamp and Majozi (2011)	6	63720	0	140		0.2	114	538	1223
	7	222840	90	130		0.3	133	631	1438
Example 5.1- Direct and indirect heat integration									
This work	7	224000	0	0	2.183,80.908	251	150	415	1453
Stamp and Majozi (2011)	6	64000	0	0	1,20	372	126	629	1560
	7	224000	0	0	3.89,76.12	1318	147	736	1833
Example 5.2 – Without heat integration									
This work	8	131376	330	400		0.2	44	408	996
Stamp and Majozi (2011)	8	86517	660	300		0.2	88	619	1202
	9	131376	330	400		0.3	99	697	1356
Example 5.2 - Direct heat integration									
This work	8	138176	30	300		0.2	82	434	1124
Stamp and Majozi (2011)	8	90517	20	400		0.1	104	667	1358
	9	138176	30	300		0.2	119	749	1532
Example 5.2- Direct and indirect heat integration									
This work	8	139977	20	100	0.528,54.47	596	114	416	1352
Stamp and Majozi (2011)	8	92317	0	200	1,97.38	10783	136	764	1709
	9	139977	20	100	0.547,57.89	4907	155	860	1931

5.4.2. Example 5.2

An industrial case study presented by Stamp and Majozi (2011) is taken as example 5.2 in the present work. The STN of this example is shown in chapter 3 as Fig. 3.2. The processing units have a fixed batch size of eight tons, which is 80 % of the design capacity. Table 3.3 of Chapter 3 shows the scheduling data. Tables 5.5 and 5.6 show the heat integration data. The computational results for the three different operational scenarios described in example 5.1 are presented in Table 5.4. The proposed STN represented unit specific event model outperforms the SSN based single time grid model of Stamp and Majozi (2011) in terms of model statistics and computational performance. The Gantt chart for the third operational scenario is presented in Fig. 5.6.

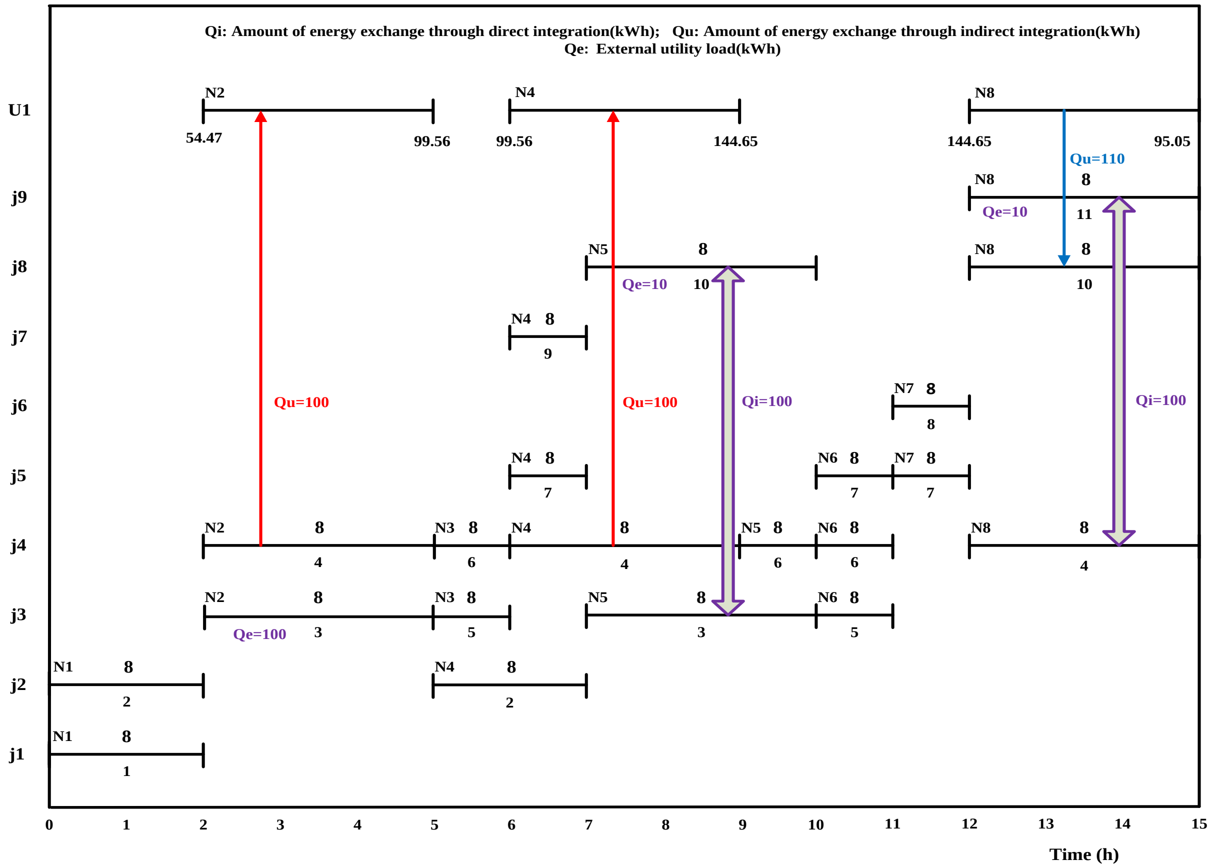


Fig. 5.6. Gantt chart for Example 5.2 with direct and indirect heat integration

Table 5.5. Stoichiometric data for the Example 5.2

Parameter	**value**
Cooling water cost (cu/Kwh)	8
Steam cost (cu/Kwh)	20
Product selling price (cu/ton)	10,000
Specific heat capacity, c_p (kJ/kg^{o}C)	4.2
Lower bound for heat storage capacity (ton)	0.2
Upper bound for heat storage capacity (ton)	1
Minimum temperature difference (^{o}C)	5
Lower bound for heat storage temperature (^{o}C)	20
Upper bound for heat storage temperature (^{o}C)	180

Table 5.6. Heating/Cooling requirements for the Example 5.2

Task(i)	**Type**	**Operating temperature(^{o}C)**	**Heating/Cooling requirement (kWh)**
Reaction2	Exothermic	150	100 (cooling)
Evaporation	Endothermic	90	110 (heating)

The effect of the amount of thermal fluid on its initial temperature and net profit is presented in Fig. 5.7. For this example the maximum net profit of 139977 cu has been observed at 0.528 ton of thermal fluid and initial temperature of 54.47 °C. At these operating conditions, the process pinch is observed at 9 hours as well as 15 hours as highlighted in Fig. 5.8. As the amount of thermal fluid increases beyond 0.528 ton, the initial temperature increases, so that the ΔT_{min} = 5 °C is maintained at 9 hours for all the amounts of thermal fluid. For all other heat exchange matches, the temperature approach is greater than 5 °C.

The above results confirm that the same optimal solution can exist at different sets of amount of thermal fluid and initial temperature. In this work, the optimal values of the amount of thermal fluid and initial temperature are calculated based on the design of the heat integration network at process pinch. This alternate approach gives more insight into the simultaneous scheduling and heat integration of batch plants.

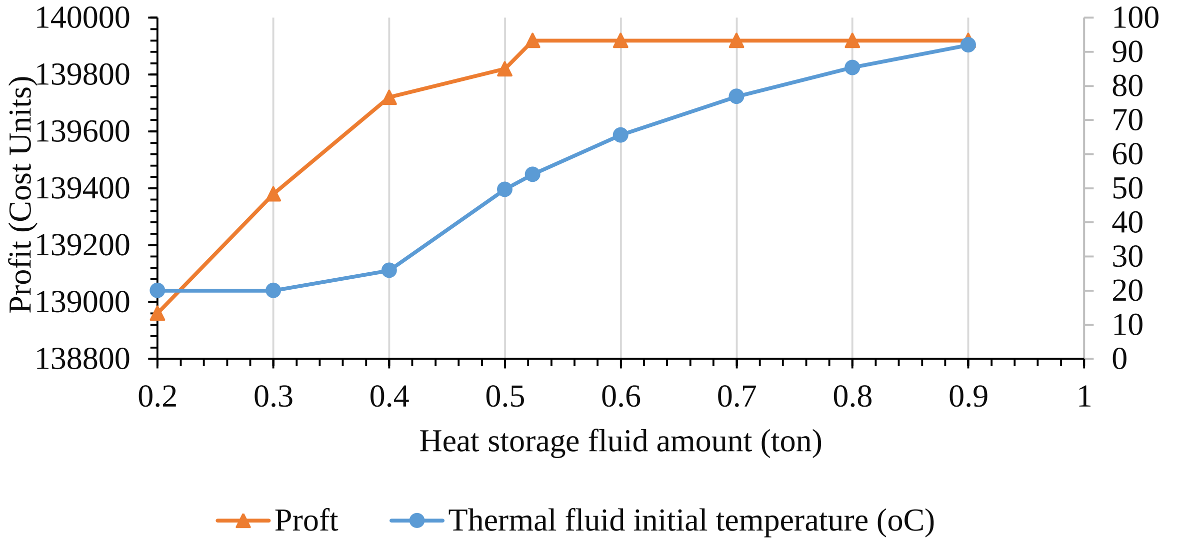


Fig. 5.7. Effect of amount of thermal fluid on net profit and initial temperature

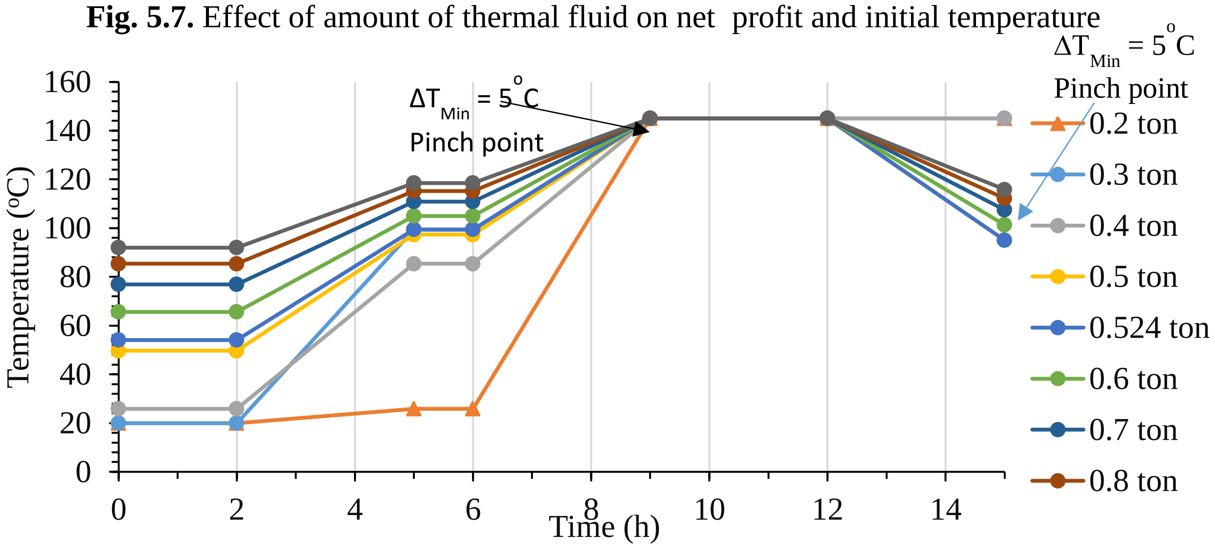


Fig. 5.8. Time dependent temperature profile for different amounts of thermal fluid

5.4.3. Example 5.3

This example was first presented by Papageorgiou et al. (1994), highlighting the advantages of direct heat integration. Recently, Sebelebele and Majozi (2017) extended this example to investigate the indirect heat integration scenario by considering design and optimization of heat storage vessels. The capital cost of the storage vessel was included in the model and its effect was evaluated on overall profit. Fig. 3.1 in Chapter 1 represents the STN diagram of this process. Table 5.7 shows the scheduling data, which is directly adopted from Sebelebele and Majozi (2017). The processing task's operating temperatures and heat capacities are given in Table 5.8.

Table 5.7. Scheduling data for the Example 5.3

Unit(j)	Task(i)	Processing Time	capacity (kg)		States	Storage Capacity(kg)	Initial Amount(kg)	Price or Cost(cu)
			Min	Max				
Reactor(j1)	Reaction	2	15	60	S1	1000	1000	0
Reactor(j2)		2	15	60	S2	1000	1000	0
Filter (j3)	Filtration	1	8	80	S3	50	0	0
Filter (j4)		1	8	80	S4	50	0	0
Distiller(j5)	Distillation	2	0	140	S5	1000	0	0
					S6	1000	0	120
					S7	1000	0	120
					Hot utility			1 cu
					Cold utility			0.02 cu

Table 5.8. Heat integration data for the Example 5.3

Task(i)	Unit(j)	Target Temperature(^{o}C)	Supply Temperature(^{o}C)	Specific heat capacity, c_p(kJ/kg^{o}C)
Reaction	Reactor(j1)	70	100	3.5
	Reactor(j2)			
Distillation	Distiller(j5)	80	65	2.6

In the present work, this example has been solved using the heat integration data from Sebelebele and Majozi (2017) (referred as S&M). While performing the computations, the following difficulties were faced, with respect to the heat integration data, provided by S&M.

i. Units of utility costs were vague, they were just reported as 1.0 cu for hot utility and 0.02 cu for cold utility. In the absence of a verifiable cross reference, the costs are taken as 1.0 cu/kJ and 0.02 cu/kJ.

ii. Details of thermal fluid are not mentioned by S&M. For our calculations, water is considered as thermal fluid with the following specifications: heat capacity 4.2 kJ/kg ^{o}C; temperature range 20 ^{o}C to 160 ^{o}C; minimum and maximum capacity 0 kg and 1000 kg respectively.

iii. For calculation of storage vessel costs, the data given by S&M (fixed cost 48000 cu and variable cost 280000 cu/kg) appeared to be erroneous, as the results reported could not be verified using these values. To cross check these values, the reference cited by S&M for these values, Li and Chang (2006) was referred. The values reported by this reference are fixed cost of 48000 cu and variable cost of 280000 cu/m^3 (The difference in units for variable cost may be noted). The results of S&M work could be verified with these values and hence these values are used for our calculation.

  Fig. 5.8 in S&M work represents the Gantt chart for scenario of direct and indirect heat integration with three heat storage vessels. In this work, the same Gantt chart is reproduced as Fig. 5.9. From the task alignment visuals of the Gantt chart, it can be seen that there are no direct heat integration matches. Also, the computational results presented in S&M work state that the requirement of external utilities is zero, thus indicating that energy requirement is met by storage vessels. The Gantt chart shows that the energy requirement for the distillation tasks was met by the third storage vessel only. Hence it is expected that the temperature of the vessel must decrease with time, when there is exchange of energy. However, the results presented by S&M were not consistent with this. As can be seen from Fig. 5.10 the temperature of third storage is constant from 3 to 5 hours during which period there was an energy exchange.

iv. Further, the S&M model failed to handle the real time storage violations. Fig. 5.9 shows the Gantt chart of S&M in which the storage profiles of intermediate material states have been incorporated by us. It can be seen that the storage of S4 is 61.6 kg during the time horizon of 5 to 7 hours while the maximum storage capacity is only 50 kg. This inconsistency would have resulted due to the absence of a constraint on intermediate storage capacity.

Keeping the above in mind, computations were carried out with the proposed model to address different scenarios, viz., a) scheduling without heating and cooling loads, b) use of external utilities for heating and cooling loads, c) direct heat integration, d) direct and indirect heat integration with a single storage vessel, e) direct and indirect heat integration with two storage vessels, f) direct and indirect heat integration with three storage vessels. In case of direct or indirect heat integration, the deficit energy demand for standalone and heat integrated tasks is compensated by using external utilities. Table 5.9 shows the heat storage vessel and utility data used for the computations.

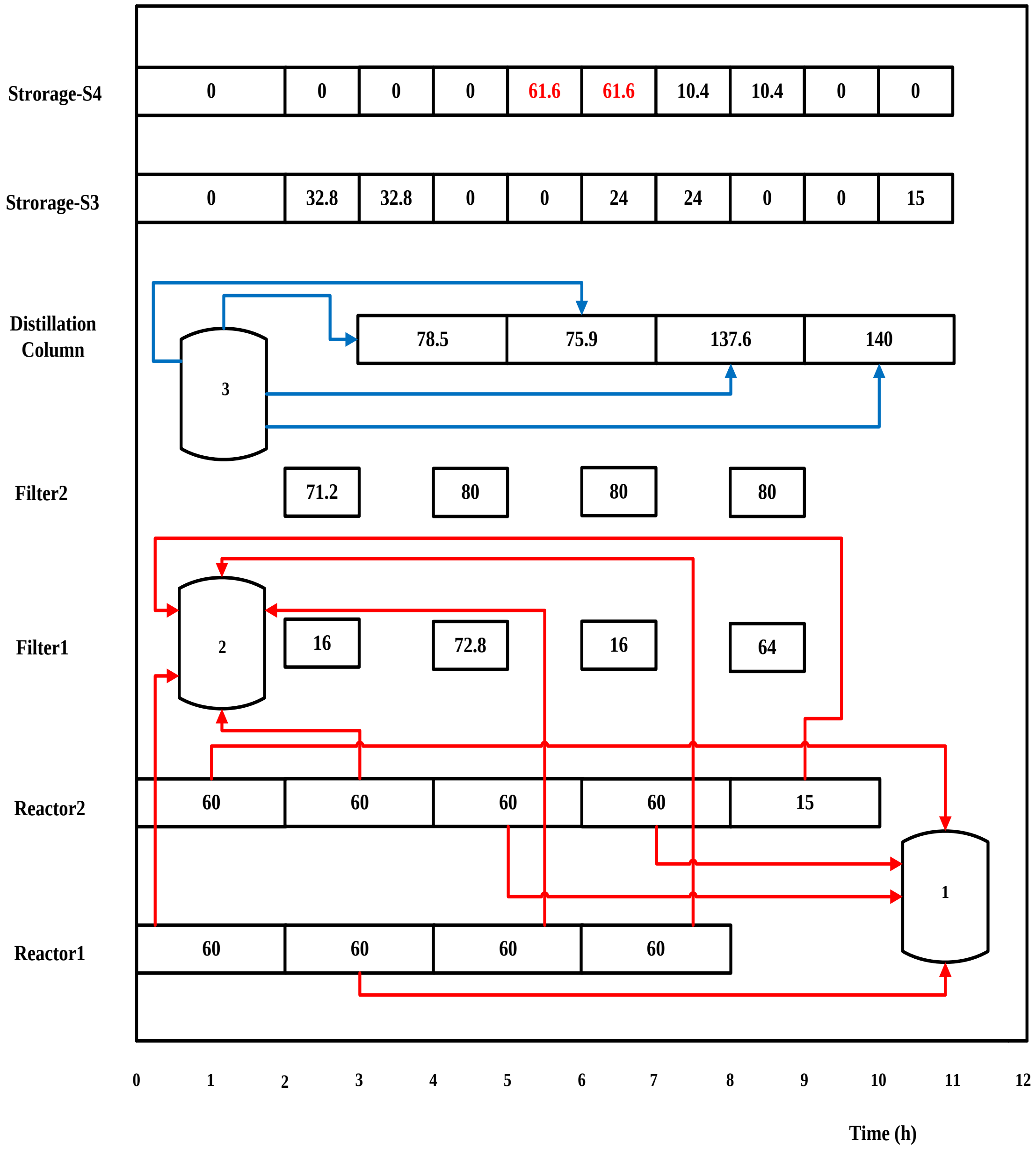


Fig. 5.9. Gantt chart for Example 5.3 with indirect heat storage (From Sebelebele and Majozi(2017))

The above defined scenarios are systematically investigated and computational results are presented in Table 5.10. For the scheduling problem without utilities (Scenario (a)) the proposed model resulted in the optimal value of 34.2 x 10^6 cu with maximum product rate of 36 kg/h which is similar to S&M model. This scenario gives the best possible production schedule because of the absence of utility requirement. As expected, the process has minimum profit when the total energy demand is met from the external utility resources as shown in Table 5.10- Scenario (b). From the Gantt chart it is seen that this net profit is obtained at the maximum product rate of 36 kg/h, as expected. However, the external utility cost reduced the overall profit to minimum value.

Table 5.9. Heat storage vessel and utility data for the Example 5.3

	Example 5.3
Parameter	**Value**
Cost function exponent	0.6
Interest rate (%)	15
No. of years(yr)	3
Operational time (hr/yr)	7920
Fixed cost of storage vessel (cu)	48000
Variable cost of storage vessel (cu/m^3)	280000
Cold utility cost (cu/kJ)	0.02
Hot utility cost (cu/kJ)	1
Selling price of the final product (cu/kg)	120

As the direct heat integration feature is incorporated, a significant improvement in net profit has been observed. The model required 9 event points and Δ*n* =1 and resulted in 33.6 x 10^6 cu net profit. The direct heat integration feature (Scenario (c)) enhanced the net profit by 50 percent as compared to the Scenario (b) as shown in Table 5.10. This solution emphases the importance of direct heat integration. Fig. 5.11 shows the Gantt chart for this case with four direct heat integration matches.

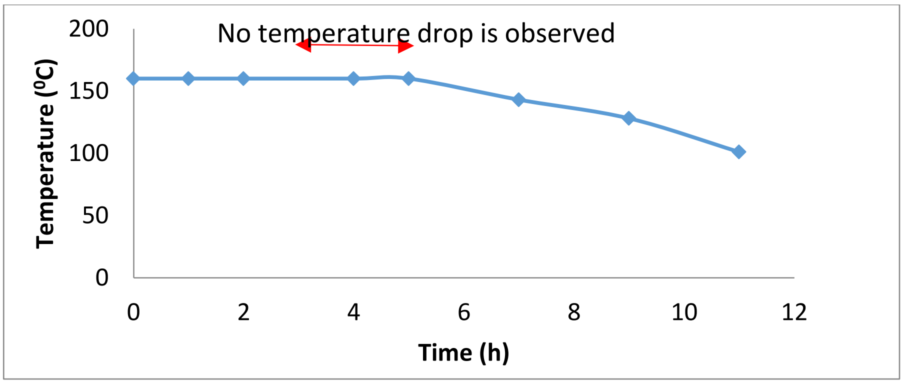


Fig. 5.10. Temperature profile of storage unit three (From Sebelebele and Majozi (2017))

When the indirect heat integration feature is incorporated along with direct heat integration, the external utility demand is reduced. For the process with single heat storage vessel (Scenario (d)), the proposed model reported an optimal value of 33.9 x 10^6 cu, whereas S&M reported 33.5 x 10^6 cu. In the present work, initial temperature of the storage vessel is 20^{o}C and it has been used as heat sink. All heating tasks are directly integrated with cooling tasks, thus eliminating the requirement of thermal fluid at high initial temperature. Contrary to this, S&M required high initial temperature thermal fluid for use as a heat source for distillation tasks. Consequently, the total amount of external utilities requirement is less in the present work as compared to S&M. The computational results presented in Table 5.10 - Scenario (d) highlight the advantage of direct heat integration in design and optimization of single heat storage vessels.

Table 5.10. Computational results for Example 5.3

	Events	Profit (c.u.)	External Hot Utility (MJ)	External Cold Utility (MJ)	Thermal oil amount (kg), Initial Temperature (^{o}C)	Annualized capital cost (cu)	CPU time(s)	Binary variables	Continuous variables	Constraints
Example 5.3										
Scenario (a): Scheduling without heating and cooling loads										
This work	6	34.2 x 10^6	--	--	--	--	0.04	20	150	302
	Scenario (b) Without heat integration									
This work	6	22.4 x 10^6	16.8	50.4	--	--	0.1	20	150	302
	Scenario (c) With direct heat integration									
This work	9 (Δn=1)	33.6 x 10^6	0	42.1	--	--	891	103	313	836
	Scenario (d) Direct & indirect heat integration with one heat storage vessel									
This work	9 (Δn=1)	33.9 x 10^6	0	16.7	112.5, 20	23057	9562	126	377	1226
	Scenario (e) Direct heat integration & indirect heat integration with two heat storage vessels									
This work	9 (Δn=1)	34.1 x 10^6	0	4175	42.8, 20 112.5, 20	22142 23057	14327	153	441	1615
	Scenario (f) Direct & indirect heat integration with three heat storage vessels									
This work	6	34.1 x 10^6	0	0	Unit1-112.5, 20 Unit2-112.5, 20 Unit3-31.9, 160	23057 23057 21953	7689	96	312	1074

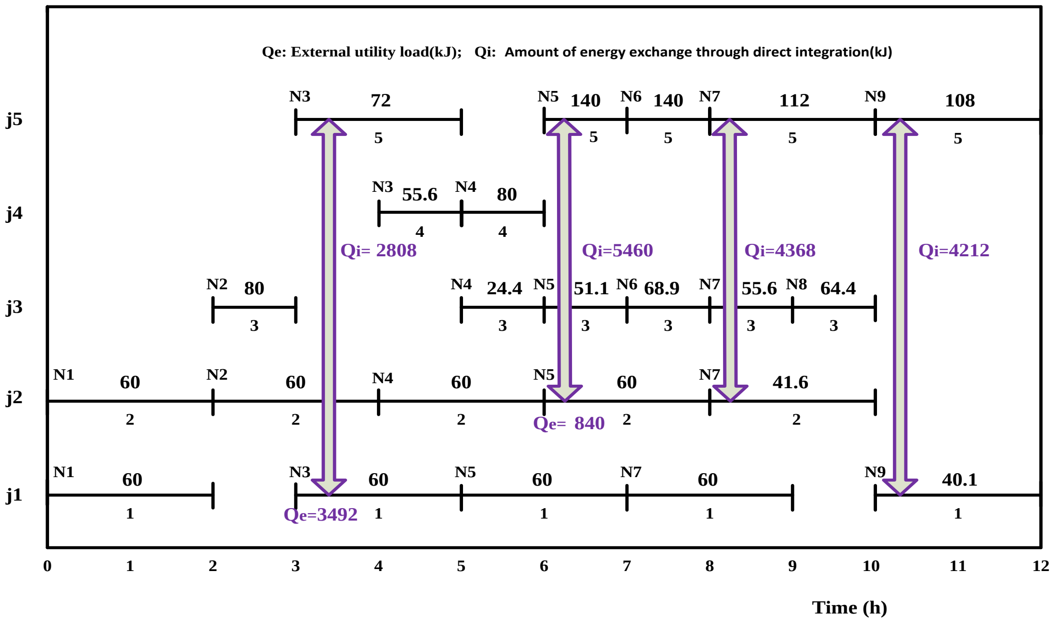


Fig. 5.11. Gantt chart for Example 5.3 with direct heat integration

The process with two heat storage vessels results in the maximum net profit of 34.1 x 10^6 cu and the computational results are presented in Table 5.10- Scenario (e), showing the optimal operating conditions of the two heat storage vessels and associated annualized capital costs. Fig. 5.12 shows the Gantt chart for this case. As highlighted in the Fig. 5.12, the proposed framework is able to capture the advantage of direct and indirect heat integrations without any prejudice, unlike S&M. S&M avoided the direct heat integration possibilities with multiple heat storage vessels, giving the reason of 'imposing stringent time constraints on the tasks'. The present model is able to successfully handle these limitations.

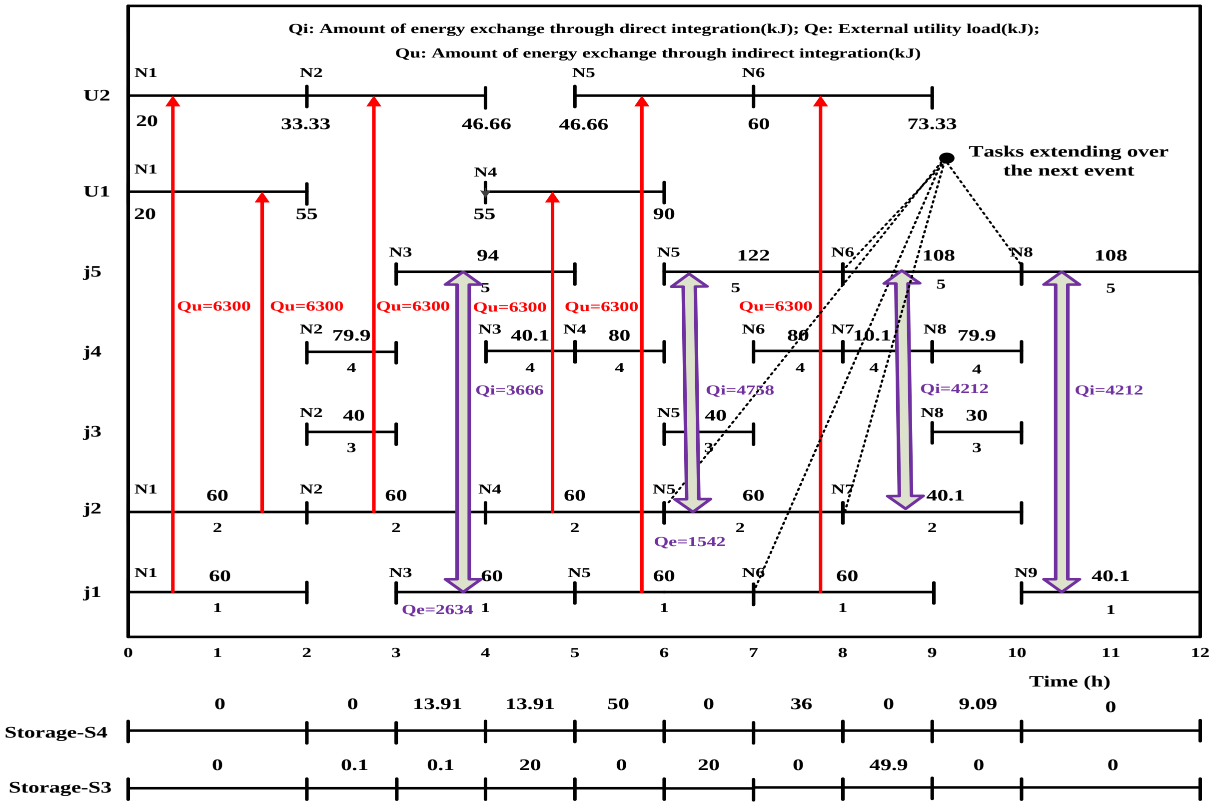


Fig. 5.12. Gantt chart for Example 5.3 with two heat storage vessels

The process with the three heat storage vessels does not require any external utilities and the computational results presented in Scenario (f) show the optimal operating conditions of the three heat storage vessels and associated annualized capital costs. Fig. 5.13 shows the Gantt chart for this case study. Both Scenarios (e) and (f) result in the same optimal value, however only two heat storage vessels are needed in Scenario (e) where as three vessels are required in Scenario (f). This reduction in the requirement of heat storage vessels reinforces the advantage of direct heat integration. Further, as highlighted in Fig. (5.12) and (5.13), the proposed model accurately monitored the storage of intermediate material states and thermal fluid temperatures on real time scale. This is an additional advantage of the present model, as S&M failed to address the real time violations as explained above in difficulties iii and iv.

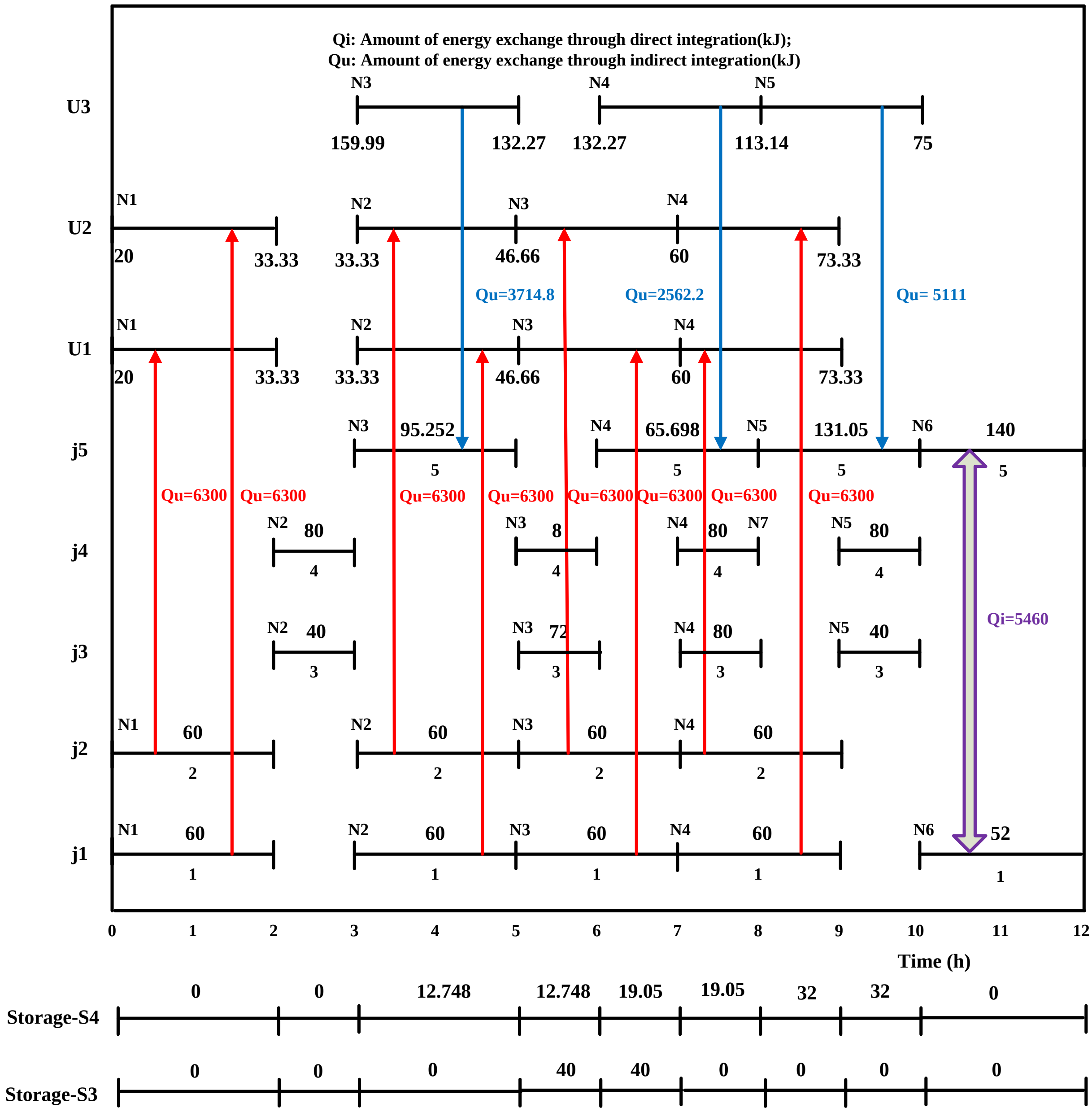


Fig. 5.13. Gantt chart for Example 5.3 with three heat storage vessels

5.5. Conclusion

In this work, a simplified unit specific event based framework is proposed for direct and indirect heat integration of batch plants with design and optimization of heat storage vessels. Different modelling issues such as task alignments, energy balances and design of heat storage vessels are precisely handled with minimum number of equations and variables. Unlike the model by Sebelebele and Majozi (2017), the proposed framework does not compromise the direct heat integration possibilities, while exploring the indirect heat integration.

The following are the conclusions drawn from the computational results:

- In the design of a single heat storage vessel, the net profit is observed to be constant beyond the optimal amount of thermal fluid. (It may be noted that the thermal fluid cost is not considered for calculating net profit.)
- As the thermal fluid amount increases beyond the optimal value, there is a change (increasing or decreasing) in initial storage vessel temperature to facilitate the network design at pinch point.
- For the first two examples, the proposed STN represented unit specific event model outperforms the SSN based single time grid model of Stamp and Majozi (2011) in terms of model statistics and computational performance.
- The proposed framework effectively handled the design and optimization of multiple storage vessels using active task concept.
- The computational results of example 3 highlight the advantage of direct heat integration in design and optimization of multiple heat storage vessels.
- The judicious use of direct and indirect heat integration possibilities reduced the requirement of heat storage vessels to two, as compared to three reported by Sebelebele and Majozi (2017).

CHAPTER 6

LONG TERM SCHEDULING AND HEAT INTEGRATION OF BATCH PLANTS: DIRECT AND INDIRECT HEAT TRANSFER USING STORAGE VESSELS

Long term scheduling and heat integration of batch plants: Direct and indirect heat transfer using storage vessels

In batch process scheduling, size of the mathematical formulation increases with operational time. Based on the time horizon considered, the scheduling problems are classified into three types: (i) short term scheduling (time horizon is in days), (ii) medium term scheduling (time horizon is in weeks), (iii) long term scheduling (time horizon is in months). Rigorous deterministic modelling approaches are available in the literature for handling short term scheduling of batch plants with different operational features. These modeling approaches are found to be inefficient for solving long term scheduling problems, because as the time horizon increases the size of the mathematical model becomes intractable.

Decomposition techniques are preferred over deterministic modelling approaches to solve long term scheduling problems. Cyclic scheduling is one of the popular decomposition techniques to effectively handle the long term scheduling problems. In the cyclic scheduling, the time horizon is divided into multiple sub sections where the operations are identical in each section. The sub section with short time horizon and different operational features can be effectively scheduled using rigorous process scheduling models.

In this chapter a rigorous Unit Specific Event Based model (USEB) is proposed for optimal utilization of direct and indirect heat integration possibilities in long term scheduling of batch processes. Using the cyclic scheduling concept, different features of direct and indirect heat integration possibilities considering design and optimization of heat storage vessels are accurately modelled.

6.1. Problem statement

The problem considered in this chapter is long term scheduling with simultaneous heat integration. The data given for this case is as follows: (i) process network, material state production and consumption, stoichiometry, batch processing times, time horizon, selling price of final products and utility cost. The aim of this study is to design an optimal production schedule for the batch process with long operational time horizon. The following assumptions are considered: zero unit wait, negligible material transfer times, heat exchanger capital cost is not considered, no unit failures, constant batch process times and utility requirement is independent of batch size.

Using the cyclic scheduling concept, the long time horizon is divided into sub intervals (cycles) of equal duration. The optimal duration of a cycle is calculated by formulating multi-objective optimization problem considering the following objectives: profit maximization and cycle time minimization. The objective function is sensitive to the following key decision variables: upper and lower limits for cycle time, external utility cost, task start and end times, batch processing amounts and storage capacity.

In this problem the time horizon is divided into three periods: initial period (start-up period), cyclic period and final period. The required amounts of intermediate material states at the beginning of each cycle are produced in the previous cycle. In the initial period the required amounts of intermediates for the first cycle are produced. In the final period the leftover intermediates in the last cycle are utilized. After scheduling the cyclic period, the initial period is solved as make-span minimization problem considering the intermediate states' initial demand at the start of the first cycle. The same initial period is again solved for profit maximization by considering the intermediate material states' demand and the corresponding time horizon calculated in make-span minimization. The final period is solved as profit maximization problem for the remaining time horizon after determining the time horizons of initial and cyclic periods. The mathematical formulation for cyclic scheduling and heat integration of batch plants considering the design and optimization of multiple storage vessels is presented in Section 6.2. The formulation presented in Chapter 5 is used for scheduling the initial and final periods.

6.2. Mathematical formulation

In the present chapter, the main objective is to optimize the use of direct and indirect heat integration in batch plants having long term scheduling horizons, as this is a scenario more often encountered in industrial applications. Towards this end, a unit specific event based framework is proposed for simultaneous cyclic scheduling and heat integration of batch plants with design and optimization of heat storage vessels. The final goal, as in case of all the other optimization problems, is to improve the net profit, considering the important industrial constraints.

In this chapter the proposed framework addresses the final research objective 2.5.4 presented in Chapter 2. To achieve the proposed objective, few independent constraints related to the cyclic scheduling and the indirect heat integration are adopted from Chapter 4 and Chapter 5 as these are similar in nature to the present proposed formulation. The newly proposed mathematical equations to integrate the cyclic scheduling with direct and indirect heat integration are presented below.

6.2.1. Objective Function

The linear objective function presented in equation (6.1) evaluates the net profit by deducting the external utility costs from product revenue. The objective function in constraint (6.2) represents the average profit per hour, where the cycle time is considered as a variable and will be calculated from the specified time horizon range.

$$Maxprofit\ \ Z = \sum_{s \in S^p} price(s) \left(\sum_{n1=N} ST(S,n1) + \sum_{i \in I_s^p} \rho_{is} \sum_{\substack{n2 \in N \\ n1-\Delta n \le n2 \le n1}} b(i,n2,n1) \right)$$

$$- \sum_{i \in I_h} \sum_{n1=1}^{N} \left(c_{uh} qhi(i,n1) \right) - \sum_{i \in I_c} \sum_{n1=1}^{N} \left(c_{uc} q(i,n1) \right), \tag{6.1}$$

$$Objective\ function = \frac{Maxprofit}{H} \tag{6.2}$$

6.2.2. Task integration

Constraint (6.3) and (6.4) ensure the possibility of one to one integration of heat source with heat sink. The active heating task at event *n1* can exchange heat with active cooling task or heat storage unit. The active task can utilize energy from external utility in the absence of direct and indirect heat integration.

$$\sum_{i1 \in I_c} x(i,i1,n1) + \sum_{u} hex(i,u,n1) \le \sum_{\substack{n2 \in N \\ n1 \le n2 \le n1+\Delta n}} w(i,n1,n2) +$$

$$\sum_{\substack{n^a \in N \\ n^a = n1 \\ n^a > N-\Delta n+1}} \sum_{\substack{n2 \in N \\ n2 \le n^a+\Delta n-N}} w(i,n1,n2), \qquad \forall\ \ i \in I_h, i \ne i1, n1 \in N \tag{6.3}$$

$$\sum_{i \in I_h} x(i,i1,n1) + \sum_{u} hex(i1,u,n1) \le \sum_{\substack{n2 \in N \\ n1 \le n2 \le n1+\Delta n}} w(i1,n1,n2) +$$

$$\sum_{\substack{n^a \in N \\ n^a = n1 \\ n^a > N-\Delta n+1}} \sum_{\substack{n2 \in N \\ n2 \le n^a+\Delta n-N}} w(i1,n1,n2), \qquad \forall\ \ i1 \in I_c, i \ne i1, n1 \in N \tag{6.4}$$

The heat integrated tasks which continue to the next cycle are modeled as active tasks at the last event. Using the wrap-up concept the extended duration is represented accurately at the beginning of same cycle. This concept is accurately modelled using the task continuity over multiple events, which is represented using Δn. Constraints (6.5) avoids the duplicate heat integration for the task *i* at the start of the cycle, if it is heat integrated and continuing from the previous cycle.

$$\sum_{i1 \in I_c, I_h} \sum_{\substack{n2 \in N \\ n2 \le nb}} hex(i1,u,n2) \le M(-w(i,n,nb) - hex(i,u,n) + 2),$$

$$\forall\ \ i \in I_c, I_h, u \in U, n \ge N - \Delta n + 1, nb \le n + \Delta n - N, \Delta n > 0 \tag{6.5}$$

6.2.3. Duration constraints

Constraints (6.6) and (6.7) enforces the finishing time of heat exchange in storage vessel *u* at last event *n* must be equal to cycle time if this heat integration is continuing to the next cycle.

$$HT^f(u,n) \ge H - M\big(2 - hex(i,u,n) - w(i,n,n1)\big),$$

$$\forall\ \ i \in I_c, I_h, u \in U, n \ge N - \Delta n + 1, n2 \le n + \Delta n - N, \Delta n > 0 \tag{6.6}$$

$$HT^f(u,n) \le H + M\big(2 - hex(i,u,n) - w(i,n,n1)\big),$$
$$\forall \; i \in I_c, I_h, u \in U, n \ge N - \Delta n + 1, n2 \le n + \Delta n - N, \Delta n > 0 \tag{6.7}$$

Constraints (6.8) to (6.11) align the starting and finishing times of heat integrated tasks continuing from the previous cycle. Constraints (6.8) and (6.9) align the finishing times of wrap-up tasks at event *n1*. Constraints (6.10) and (6.11) enforces the start time of wrap-up tasks at event *n1* as zero.

$$HT^f(u,n1) \ge T^f(i,n1) - M\big(2 - hex(i,u,n) - w(i,n,n1)\big),$$
$$\forall \; i \in I_c, I_h, u \in U, n \ge N - \Delta n + 1, n2 \le n + \Delta n - N, \Delta n > 0 \tag{6.8}$$

$$HT^f(u,n1) \le T^f(i,n1) + M\big(2 - hex(i,u,n) - w(i,n,n1)\big),$$
$$\forall \; i \in I_c, I_h, u \in U, n \ge N - \Delta n + 1, n2 \le n + \Delta n - N, \Delta n > 0 \tag{6.9}$$

$$HT^s(u,n1) \ge 0 - M\big(2 - hex(i,u,n) - w(i,n,n1)\big),$$
$$\forall \; i \in I_c, I_h, u \in U, n \ge N - \Delta n + 1, n2 \le n + \Delta n - N, \Delta n > 0 \tag{6.10}$$

$$HT^s(u,n1) \le 0 + M\big(2 - hex(i,u,n) - w(i,n,n1)\big),$$
$$\forall \; i \in I_c, I_h, u \in U, n \ge N - \Delta n + 1, n2 \le n + \Delta n - N, \Delta n > 0 \tag{6.11}$$

6.2.4. Energy balance constraints

In the cyclic scheduling, the operating conditions at the starting and finishing of the cycle must be same. Constraints (6.12) and (6.13) calculate the amount of external cold or hot utility required to cool or heat the thermal fluid to initial state.

$$eqlcu(u) \ge wt(u)C_p(u)\left(TT^f(u,N) - TT^s(u,n)\right),$$
$$\forall \, u \in U, n \in N, n = 1 \tag{6.12}$$

$$eqlhu(u) \ge wt(u)C_p(u)\left(TT^s(u,n) - TT^f(u,N)\right),$$
$$\forall \, u \in U, n \in N, n = 1 \tag{6.13}$$

Constraints (6.14) and (6.15) depict the energy balance of cooling and heating tasks. In case of direct or indirect heat integration, the deficit energy demand is compensated by using external utility. In direct heat integration the amount of energy exchange is restricted to minimum energy load of the integrated tasks as represented in Constraint (6.16). Constraints (6.17) and (6.18) align the starting times of direct heat integrated tasks.

$$qmt(i) \sum_{\substack{n1 \in N \\ n \le n1 \le n + \Delta n}} w(i,n,n1) + \sum_{\substack{n1 \in N \\ n \le n1 \le N - \Delta n + 1}} \sum_{\substack{n2 \in N \\ n2 \le n1 + \Delta n - N}} w(i,n1,n2) =$$
$$q(i,n) + \sum_u qs(i,u,n) + \sum_{i1 \in I_h} mqmt(i1,i,n), \quad \forall \quad i \in I_c, n \in N \tag{6.14}$$

$$qmt(i) \sum_{\substack{n1 \in N \\ n \le n1 \le n + \Delta n}} w(i,n,n1) + \sum_{\substack{n1 \in N \\ n = n1 \\ n1 \le N - \Delta n + 1}} \sum_{\substack{n2 \in N \\ n2 \le n1 + \Delta n - N}} w(i,n1,n2) =$$
$$q(i,n) + \sum_u qs(i,u,n) + \sum_{i1 \in I_c} mqmt(i,i1,n), \quad \forall \quad i \in I_h, n \in N \tag{6.15}$$

$$mqmt(i,i1,n) \leq min\big(qmt(i), qmt(i1)x(i,i1,n)\big), \ \forall \quad i \in I_h, i1 \in I_c, n \in N \tag{6.16}$$

$$T^s(i,n) \geq T^s(i1,n) - M\big(1 - x(i,i1,n)\big), \qquad \forall \ \ i \in I_h, i1 \in I_c, n \in N \tag{6.17}$$

$$T^s(i,n) \leq T^s(i1,n) + M\big(1 - x(i,i1,n)\big), \qquad \forall \ \ i \in I_h, i1 \in I_c, n \in N \tag{6.18}$$

6.2.5. Important enhancements of the proposed framework

A unit specific event based modeling approach is proposed to handle the cyclic scheduling and heat integration of batch plants with design and optimization of multiple storage vessels. The proposed approach addresses the complete scheduling of long-term operational horizon by considering start-up, cycle and finishing periods. The start-up period takes care of intermediate material states' requirement at the beginning of first cycle and finishing period effectively utilizes the leftover intermediate states at the end of final cycle. The direct and indirect heat integration possibilities are incorporated while scheduling the start-up and final periods. The meaning of cyclic scheduling is precisely incorporated using the task wrap-up concept. The task extending to next cycle is indicated at the beginning of the cycle by incorporating task splitting over multiple events. Using the active task concept the material and energy balances for warp-up tasks are modelled with minimum number of equations. The proposed formulation does not require extra event points to align the material and energy inventories at the starting and ending of the cycle. The proposed formulation effectively handles the design and optimization of multiple storage vessels by finding the optimal number of storage vessels and calculating their sizes and initial temperatures.

6.3. Computational Results

In this chapter, two examples adopted from Stamp and Majozi (2011) are investigated to demonstrate the computational effectiveness and accuracy of the proposed formulation. The optimization solvers GAMS 24.4.1- CEPLEX and BARON are used to solve the linear and non-linear models respectively. The desktop computer consisting of Intel Xeon E5-1607 3.00 GHz processor with 8 GB RAM and Windows 7 operating system is used as a computational resource.

6.3.1. Example 6.1

This multipurpose batch process example was first discussed by (Kondili et al., 1993). Later, it has become a benchmark example in batch process scheduling area because of its complex network structure and multipurpose utilization of reactors. The performance and accuracy of numerous scheduling models were evaluated by solving this example. In this thesis, this example is first presented as motivating example in Chapter 4 and used to evaluate the computational performance of the proposed cyclic scheduling framework. The STN of this example is presented in Fig. 4.1. The scheduling data and heat integration data are presented in Table 4.1. The long term scheduling horizon is divided into three periods: initial, cyclic and final periods. Each period is evaluated by considering three operational scenarios: a) without heat integration b) direct heat integration and c) direct and indirect heat integration. The scenario (c) is further divided into the following two sub sections: (i) - scheduling with selection of heat storage vessel as an optimization variable, (ii) – scheduling by enforcing the utilization of finite number of heat storage vessels.

The cyclic period is solved by using the MINLP formulation proposed in Section 6.2. Optimal cyclic length is calculated form the specified time range of 3 to 6 hours. The mathematical model presented in Chapter 5 is used to schedule the initial and final periods. If the calculated initial and final time periods are less than the optimal cycle time, the period's duration is increased by one cycle length. Finally, the initial and final periods are also solved for profit maximization. Computational results for the three operational scenarios are presented in Table 6.1.

The cyclic scheduling solution for the process with external heating and cooling loads is presented as Case (a) in Table 6.1. As expected this scenario results in a minimum overall profit due to the use of external utilities. Improvement in the overall profit is observed when direct heat integration possibilities are incorporated in cyclic scheduling as shown in Case (b) of Table 6.1. Fig. 6.1 shows the overall Gantt chart for this scenario. For the simultaneous direct and indirect heat integration scenario, in cyclic period, both the options (i) and (ii) have resulted in the same objective value of 3441.3 c.u. per hour. In option (i), heat storage vessel is not utilized and resulted in the same overall solution as that of direct heat integrated solution presented in Case (b). In option (ii), further improvement in overall profit has been observed due to the effective utilization of storage vessels in the initial and final periods. Fig. 6.2 shows the Gantt chart for initial, cyclic and final periods for Case (c) option (ii) where indirect heat integration is handled by using one heat storage vessel.

The option (ii) is further explored by enforcing the use of two heat storage vessels. For the cyclic period, option (ii) with two heat storage vessels resulted in more product throughput than the process with single storage vessel at an optimal cycle length of 5 hours. However, both these cases resulted in the same objective value of 3441.3 c.u. per hour in the cyclic period. This is mainly due to the requirement of additional cold utility to cool the thermal fluid in heat storage vessel U1 to initial state at the end of cycle as shown in Fig. 6.3. However, the total overall profit is more in this case because of effective utilization of the two storage vessels in the initial and final periods. Fig. 6.3 shows the Gantt chart for initial, cyclic and final periods for option (ii) where indirect heat integration is handled by using two heat storage vessels.

The cyclic scheduling solution is also compared with direct solution obtained at the total time horizon of 24 hours. For scenarios (a) and (b), the direct solution resulted in better objective values than the cyclic scheduling approach, because the cyclic scheduling is a decomposition technique which always results in a near optimal solution. For simple problem instances such as scenarios (a) and (b), the direct solution is always superior than the solution of any decomposition technique. As the indirect heat integration is incorporated the problem complexity increased significantly. Thus, the direct solution by using MINLP model is inferior and not converging. Whereas, better optimal and converged results have been observed using cyclic scheduling approach as shown in Table 6.1.

6.3.2. Example 6.2

An industrial case study discussed in Chapter 3 and 4 is solved by considering the relevant cyclic scheduling data from Stamp and Majozi (2017). This industrial case study is first presented by Majozi and Zhu (2001) and later it has been used for evaluating different heat integration and process scheduling models proposed in the literature. The STN of this example is shown in Chapter 3 as Fig. 3.4. The processing units have a minimum batch size of 1.2 tons and maximum batch size of eight tons which is 80 % of the design capacity. Table 3.3 of Chapter 3 shows the scheduling data. Tables 5.5 and 5.6 of Chapter 5 show the heat integration data.

Similar to the Example 6.1, the long term scheduling horizon of 48 hours is divided into three periods: initial, cyclic and final periods. Each period is evaluated by considering three operational scenarios discussed in the Example 6.1. The cyclic period is solved by using the proposed MINLP formulation in Section 6.2. Optimal cyclic length is calculated form the specified time range of 6 to 9 hours. The mathematical model presented in Chapter 5 is used to schedule the initial and final periods. If the calculated initial and final time periods are less than the optimal cycle time, the period's duration is increased by one cycle length. Finally, the initial and final periods are also solved for profit maximization.

The computational results for the three different operational scenarios described in example 6.2 are presented in Table 6.2. From the computational results presented in Table 6.2, it is observed that the operational scenarios (b) and (c)-(i) resulted same profit per hour (16381 c.u./hour) in the cyclic period length 9 hours. The hot utility requirement is 40 kWh and cold utility requirement is zero. Fig. 6.4 shows the overall Gantt chart for scenario (b). The scenario (c)-(i) has not utilized the available storage vessel in cyclic period, because even with the utilization of one heat storage vessel there is no improvement in the cyclic solution. Further, enforcing the utilization of more storage vessel decreases the overall objective value as shown in Table 6.2 scenario (c)-(ii). In this case study, the process with direct heat integration resulted in better optimal results than the simultaneous direct and indirect heat integration scenario.

Table 6.1. Computational results from Example 6.1

	Events	Profit (c.u.)	External Hot Utility (kWh/ period)	External Cold Utility (kWh/period)	Thermal oil amount (kg), Initial Temperature (^{o}C)	CPU time(s)	Binary variables	Continuous variables	Constraints
Example 6.1									
Scenario (a). Scheduling with external heating and cooling loads									
Direct solution									
H=24h	15	70520	800	1040		54370	120	505	1256
Cyclic scheduling									
Initial H=7h	4	7645	240	320		0.01	31	135	303
Cyclic H=5 x 2	4(Δn=1)	33173	160	260		10.3	64	167	437
Final H= 7h	5	27851.5	240	270		0.2	32	133	299
Total Profit		68669.5							
Scenario (b). With direct heat integration									
Direct Solution									
H=24h	15	76702	350	580		120000[a]	240	709	1916
Cyclic Scheduling									
Initial H=9h	5	9977	120	190		0.3	80	239	610
Cyclic H=5 x 2	3	34413	30	130		10.2	48	144	306
Final H= 5h	3	29340	20	130		0.2	48	142	344
Total Profit		73730							
Scenario (c). Direct and indirect heat integration									
(i). Cyclic scheduling with selection of heat storage vessel is an optimization variable									
Initial H=7h	Same as the solution of direct heat integration								
Cyclic H=5 x 2	3	34413	30	130	Zero	862	67	177	494
Final H= 7h	Same as the solution of direct heat integration								
(ii). Cyclic scheduling with one heat storage vessel									
Direct Solution									
H=24h	15	55710	460	520	U1:0.829, 70	120000[b]	330	860	2702
Cyclic Scheduling									
Initial H=7h	4	8411	40	130	U1:0.715, 70	0.18	88	231	693
Cyclic H=5 x 2	3	34413	30	130	U1:0.715, 70	5367	67	177	494
Final H=7h	5 (Δn=1)	31121	40	90	U1:0.715, 70	0.8	142	317	1088
Total Profit		73945							
(ii). Cyclic scheduling with two heat storage vessels									
Direct Solution									
H=24h	15	32608	466	600	U1:0.11, 68.35 U2:0.166, 20	120000[c]	420	1011	3604
Cyclic Scheduling									
Initial H=7h	4	11237	50	188.6	U1:1.228, 20 U2:0.271, 122	0.4	112	270	931
Cyclic H=5 x 2	3	34413	30	123.3	U1:1.228, 20 U2:0.271, 70	120000[d]	84	210	682
Final H=7h	5 (Δn=1)	28458	40	30	U1:1.228, 20 U2:0.271, 70	1.3	172	366	1434
Total Profit		74108							

[a] Relative Gap: 0.00018%, [b]Relative Gap: 0.0034%, [c]Relative Gap: 0.0062%, [d]Relative Gap: 0.00013%

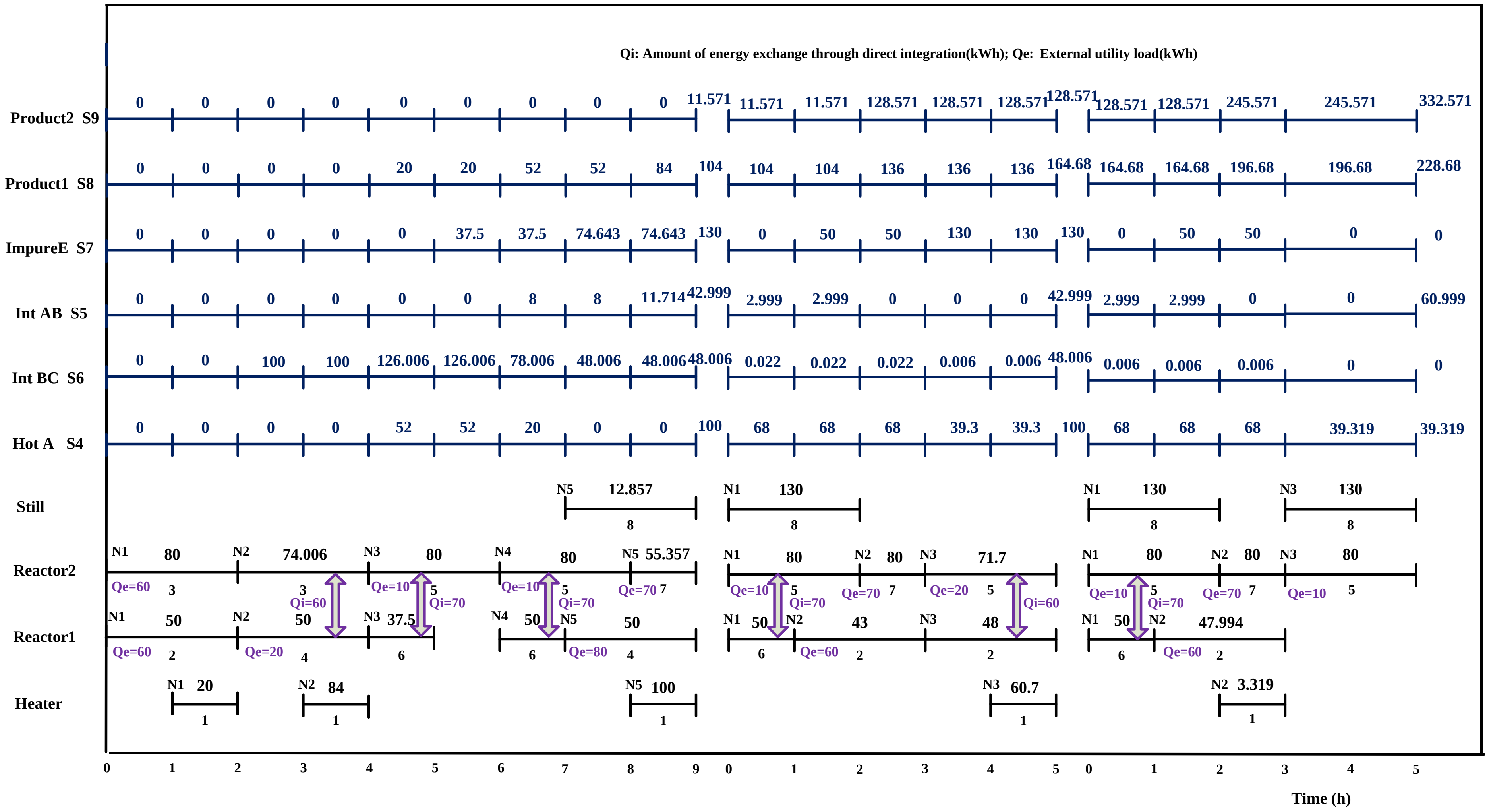


Fig. 6.1. Gantt chart for Example 6.1 with direct heat integration

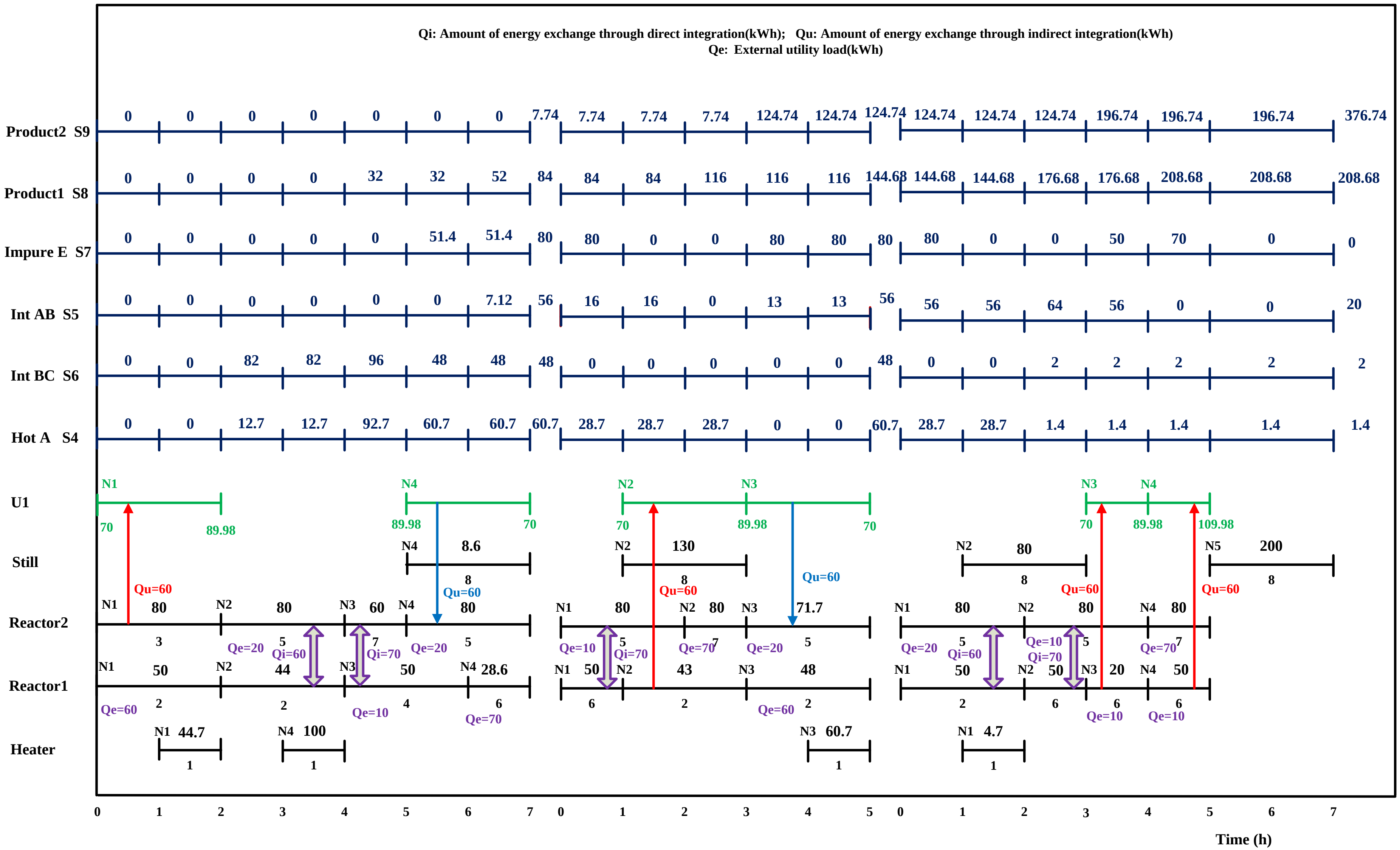


Fig. 6.2. Gantt chart for Example 6.1 with direct and indirect heat integration using one storage vessel

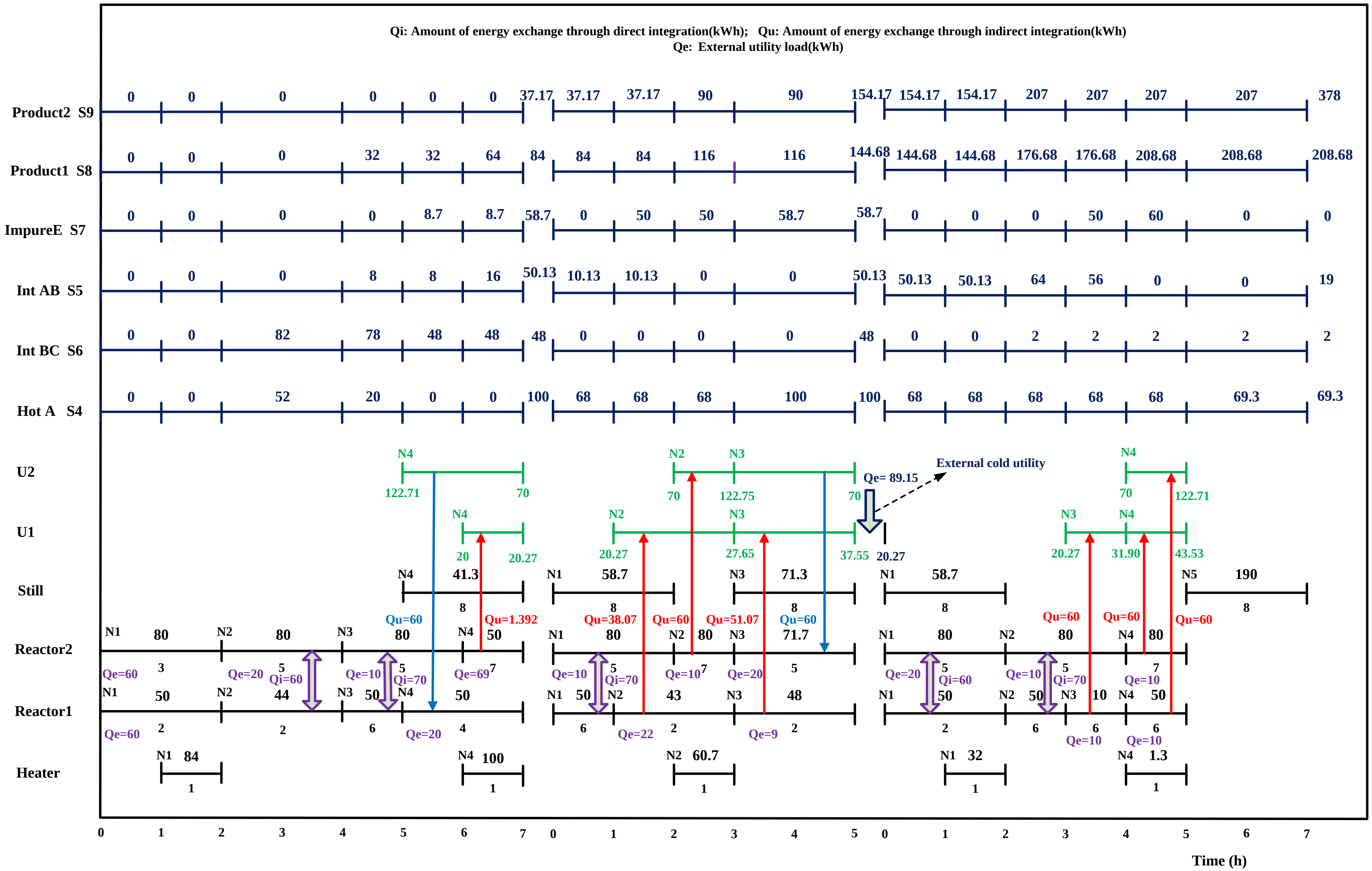


Fig. 6.3. Gantt chart for Example 6.1 with direct and indirect heat integration using two storage vessel

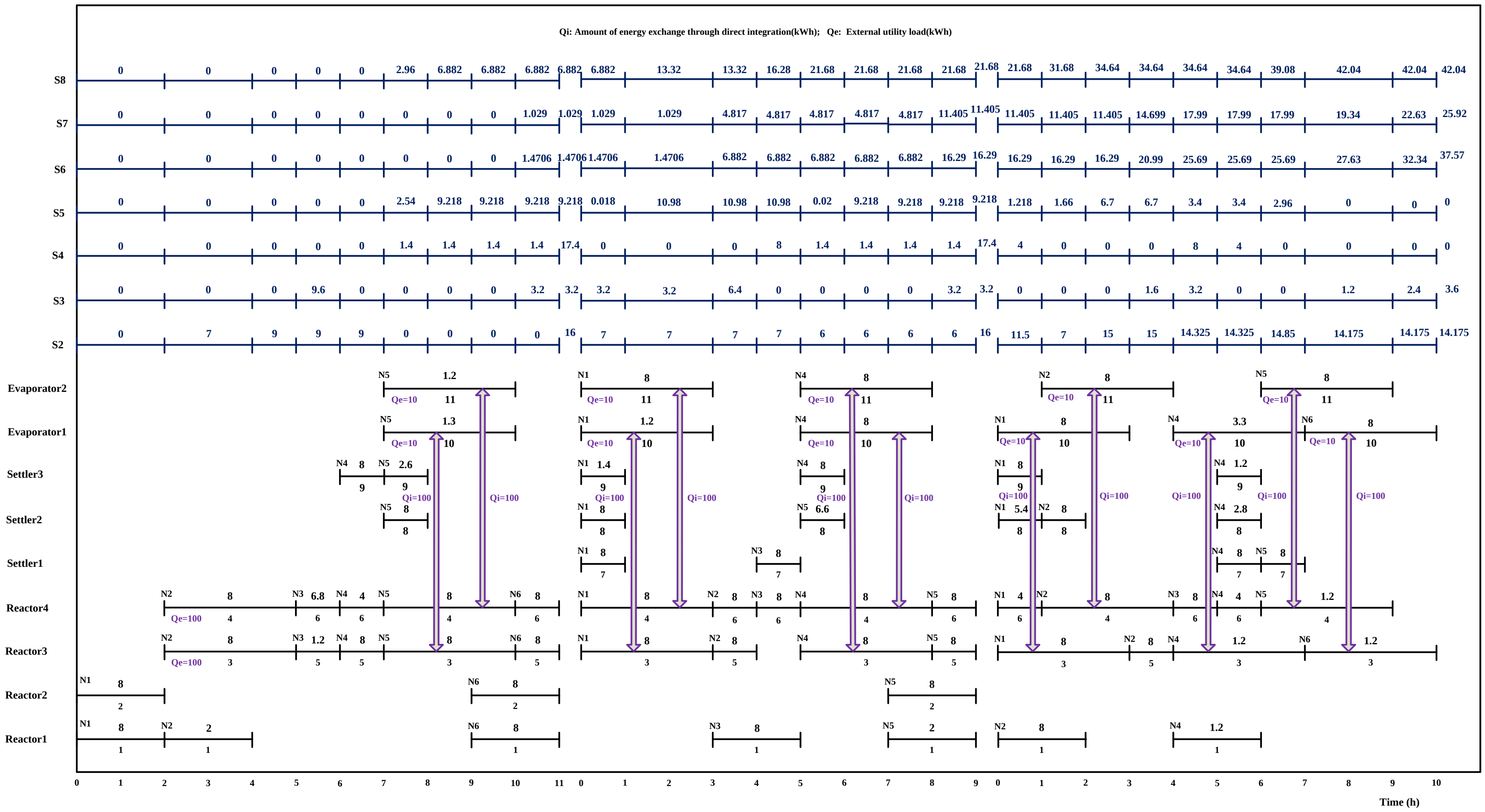


Fig. 6.4. Gantt chart for Example 6.2 with direct heat integration

Table 6.2. Computational results for Example 6.2

	Events	Profit (c.u.)	External Hot Utility (kWh/period)	External Cold Utility (kWh/period)	Thermal oil amount (kg), Initial Temperature (^oC)	CPU time(s)	Binary variables	Continuous variables	Constraints
Example 6.2									
Scenario (a): Scheduling with external heating and cooling loads									
Direct solution									
H=48h	25	660335	2000	1760		120000[a]	275	1105	3532
Cyclic scheduling									
Initial H=15h	7	9182	110	700		0.25	77	313	944
Cyclic H=9 x 2	7	272473	440	400		2836	77	313	803
Final H= 15h	9	367667	990	400		4	99	370	1228
Total Profit		649322							
Scenario (b) With direct heat integration									
Direct Solution									
H=48h	25	702535	270	400		120000[b]	375	1305	4032
Cyclic Scheduling									
Initial H=11h	6	12823	20	200		0.18	90	317	920
Cyclic H=9x3	5	442308	40	0		7.4	75	265	659
Final H= 10h	6	206531	50	0		0.6	90	313	916
Total Profit		661662							
Scenario (c) Direct and indirect heat integration with one heat storage vessel									
Option (i): Cyclic scheduling with selection of heat storage vessel is an optimization variable									
Initial	Solution is same as Scenario (b)								
Cyclic H=9x3	5	442308	40	0			96	308	881
Final	Solution is same as Scenario (b)								
Option (ii): Cyclic scheduling with one heat storage vessel									
Direct Solution									
H=48h	25	156887	250	470		120000[b]	475	1506	4816
Cyclic Solution									
Initial H= 14 h	9	16412	10	100	U1:1.5, 47.38	10.34	171	544	1702
Cyclic H=9 x 2	5	294872	40	0	U1:1.5, 110.8	91497	96	308	881
Final H= 16h	8	349579	180	0	U1:1.5, 110.8	242	152	480	1501
Total Profit		660863							

[a] Relative Gap: 0.00021%, [b]Relative Gap: 0.00021%, [c]Relative Gap: 0.0078%,

The cyclic scheduling solution is as also compared with direct solution obtained at the total time horizon of 48 hours. Similar to the computational results of example 6.1, in the absence of indirect heat integration, the direct solution resulted in better objective values than the cyclic scheduling approach. The cyclic scheduling approach resulted as the promising option over the direct solution for handling complex problems such as long term scheduling and heat integration of batch plants with direct and indirect heat integration.

6.4. Conclusion

In this work, a unit specific event based framework is proposed for simultaneous cyclic scheduling and heat integration of batch plants with design and optimization of heat storage vessels. For handling the process with long term operational horizons, a novel solution methodology is proposed which consists of cyclic, initial and final period's scheduling in sequence. In the cyclic period, the starting and ending times of all processing units usually occupies with different tasks, therefore, the probability of direct heat integration is very high. Therefore, for both case studies, no improvement in objective value is observed with the inclusion of indirect heat integration. The presented computational results highlighted the importance of direct heat integration in process industries and cyclic scheduling solution compared to the direct solution for complex and long term scheduling problems.

CHAPTER 7

CONCLUDING REMARKS AND FUTURE WORK

Concluding Remarks and Future Work

7.1. Motivation to work on process scheduling and heat integration problem

Scheduling has been an important decision-making operation in chemical industries to optimize production and design production schedules to accommodate market fluctuations. Scheduling appears in a wide range of areas: optimal utilization of shared multiproduct facilities and material transportation in chemical, Petro-chemical, pharmaceutical and specialty chemical sectors. Different scheduling aspects including storage policies, material transfer times, variable production and consumption, resource allocation, unit wait times and cyclic scheduling are well studied using different mathematical models.

Most of the chemical operations need to be carried out at specified operating conditions, in the presence of external heating or cooling. The requirement of external utilities can greatly be reduced by integrating the heat generating process tasks. Different heat integration aspects such as heat exchange between the process streams, external utilities, heat transfer area, number of heat exchangers, operational cost and capital cost are well studied by using heat integration methodologies.

Further, the increase in demand and popularity of batch plants and striving efforts to reduce the energy utilization laid a strong foundation to the development of novel modeling techniques for simultaneous batch process scheduling and heat integration. Simultaneous scheduling and heat integration is an interactive approach which can play a potential role in design of energy efficient production schedules.

Rigorous multiple time grid modelling approaches have been proposed in literature to address different operational characteristics of batch process scheduling and heat integration independently. Only a handful of research works highlighted the computational effectiveness of multiple time grid modelling approach for simultaneous scheduling and heat integration of batch plants (Lee et al (2015, 2016), Seid and Majozi (2014), Stamp and Majozi (2017), etc.). Further, the proposed models independently explored the direct and indirect heat integration possibilities. However, judicious use of simultaneous direct and indirect heat integration results in minimum utility requirement. The industrial importance of simultaneous scheduling and heat integration, along with the identified research gaps are the main motivating factors for this research topic.

7.2. Method development

For obtaining optimal solution to a given scheduling problem, unit specific event based models show computationally better performance than slot based and global event based models. However, these models are not well explored for implementation of direct and indirect heat integration possibilities in simultaneous cyclic scheduling and heat integration.

Hence, the main objective of this work is development of robust unit specific event based model for simultaneous cyclic scheduling and heat integration of batch plants using direct and indirect heat integration possibilities. The four working chapters in this work describe the systematic developments in modelling framework to achieve the above objective. Firstly, the scheduling model proposed by Vooradi and Shaik (2012) is extended to handle the simultaneous scheduling and direct heat integration possibilities. The direct heat integration is handled by writing the energy balance equations, integration of heating and cooling task's start times and finish times. In utility balance equations, the linearization of bilinear terms is handled by using Glover transformation with minimum number of variables and constraints. Secondly, the proposed formulation is extended to handle simultaneous cyclic scheduling and direct heat integration of batch plants. The framework uses three index binary (*w(i,n1,n2))* and continuous (*b(i,n1,n2)*) variables. These variables can easily handle the task continuity over multiple events and have the advantage in finding the optimal solution. Using the concept of active task, the proposed formulation can track the inventory of intermediates available at the cycle starting time without the need of a dedicated event point. The storage of intermediate states and real time storage violations are monitored using two auxiliary constraints. The active task concept and three index binary variables integrated the cyclic scheduling and process scheduling model equations on a unified framework. This generic cyclic scheduling framework allowed the simultaneous direct heat integration with inclusion of independent energy balance and allocation constraints.

Thirdly, the framework is further extended to handle both direct and indirect heat integration by using a set of simple energy balance constraints. The proposed framework avoids the need of bilinear and trilinear terms for linearizing the indirect heat integration modelling aspects. The heat integration framework consists of allocation constraints, energy balance constraints, thermal fluid temperature constraints and heat exchange duration constraints. Finally, a rigorous framework is proposed to address the complete scheduling of long-term operational horizon by considering start-up, cycle and finishing periods. The start-up period takes care of intermediate material states' requirement at the beginning of first cycle and finishing period effectively utilizes the leftover intermediate states at the end of final cycle. The meaning of cyclic scheduling is precisely incorporated using the task wrap-up concept. The task extending to next cycle is indicated at the beginning of the cycle by incorporating task splitting over multiple events.

7.3. Limitations of the proposed formulations

In order to have a fair comparison with the proposed models in the literature, the following assumptions have been considered in this work: negligible material transfer times, no unit failures, batch processing time is linearly related with batch size, pre-processing material waiting is not allowed, no intermediate demand due dates, zero intermediate storage cost, capital and operating cost of heat exchangers are not considered. The number of event points required to obtain optimal solution is estimated using trial and error method.

Further, the proposed framework did not consider the following operational features while modelling: manpower resources, raw material and end product delivery logistics, process safety, uncertainties associated with raw material availability, product demand, unit failures and utility availability.

7.4. Research outcomes

In this work, the unit specific event based scheduling modelling framework is systematically extended to handle simultaneous cyclic scheduling and heat integration.

The following are the key outcomes drawn from the proposed theoretical developments:

- A three index unit specific event formulation is proposed to handle simultaneous scheduling and direct heat integration of batch plants. In comparison to Chen and Chang (2009) model, the proposed formulation is found to be consistently require minimal number of event points, continuous variables and binary variables. In Example 3.2 without heat integration case study the proposed model reported better objective value of 1081.7 rcu as compared to the 1071 rcu reported in the literature.
- A unified formwork is proposed for short term and/or cyclic scheduling of batch plants. The proposed unified framework will reduce to simple short-term scheduling model in the absence of cyclic scheduling. The proposed formulation integrates the cyclic scheduling and process scheduling model equations on a unified framework, whereas Wu and Ierapetritou (2004) model appended cyclic scheduling constraints to short term scheduling model. Hence, the size of the proposed model (in terms of model equations, continuous variables and binary variables) is considerably less than Wu and Ierapetritou (2004) model. The computational results presented in Chapter 4 highlighted that the proposed formulation is superior in terms of model statistics than the Wu and Ierapetritou (2004) model. The unified framework is also

extended to handle simultaneous scheduling and direct heat integration. The size of the proposed unit specific event-based formulation is less than the global event-based model proposed by Chen and Chang (2009). The computational results presented in Chapter 4 shows that better optimal results can be obtained with cycle time considered as a variable.

- A new three index unit-specific event-based model is proposed for process scheduling heat integration of batch plants with design and optimization of heat storage vessels. Different modelling issues associated with process scheduling and indirect heat integration are precisely handled with minimum number of equations and variables. The proposed framework does not compromise the direct heat integration possibilities, while exploring the indirect heat integration. The judicious use of direct and indirect heat integration possibilities reduced the requirement of heat storage vessels to two, as compared to three reported by Sebelebele and Majozi (2017).
- A rigorous unit specific event based framework is proposed for simultaneous cyclic scheduling and heat integration of batch plants with design and optimization of heat storage vessels. The proposed solution methodology consists mainly scheduling of cyclic, initial and final periods in a sequence. The proposed framework with task wrap-up concept can effectively utilize the direct heat integration possibilities along with indirect heat integration in cyclic period. As the problem complexity increases, the direct solution by using MINLP model is inferior which did not converge where as better optimal and converged results have been observed using the proposed rigorous model.

7.5. Impact of research outcomes on society

Most of the chemical industries are known to be energy intensive manufacturing units, which include petrochemicals, pulp and paper, basic chemicals, refining, nonferrous metals, iron and steel, nonmetallic minerals and food. Chemical industries are the largest consumer of energy compared with all other energy intensive industries. With the rapid industrialization and growth in population, the demand for energy is increasing continuously. However, because of the cost and availability, the most used source of energy is non-renewable, which also has the largest effect on the environment because of the emission of CO_2.

The objectives of simultaneous scheduling and heat integration models such as maximization of profit, minimization of makespan and external utility requirement results in better operational schedules for multiproduct and multipurpose batch plants. This ultimately reduces the external energy requirement and cost of the final product. Therefore, the reduction in energy requirement leads to low CO_2 emission and helps the society to have green environment.

7.6. Scope of future work

- The proposed concept of one to one integration of heat source with heat sink needs to be further explored to one to many which has significant potential to further minimize the external utility requirement.
- The proposed simultaneous scheduling and heat integration models need to be further explored by considering other important features of batch process industries such as intermediate due dates, unit wait times, material transfer times and uncertainties such as unit failures, material availability, demand and price fluctuations.
- The performance of the proposed models are evaluated by using the benchmark examples from the literature. Despite the proposed improvements it is still a challenging mission to solve large scale and complex industrial scheduling problems. A suitable real time industrial problem needs to be identified and studied using the proposed formulations.
- The proposed scheduling models need to be integrated with planning and control models to improve productivity.

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Appendices

Appendix A: Stamp and Majozi (2011) Model

Allocation Constraints:

$$\sum_{s \in S_j^{eff}} y(s,j,p) \leq 1\,, \quad \forall \;\; j \in J, p \in P \qquad (A1)$$

Capacity Constraints:

$$V_j^{min}\, y(s,j,p) \;\leq \sum_{\substack{sa \in S_j^{in} \\ \rho_{in}(s,sa)}} mu\,(sa,j,p) \leq V_j^{max}\, y(s,j,p), \quad \forall \; j \in J, s \in S_j^{eff}, p \in P \qquad (A2)$$

Material Balances:

$$\sum_{\substack{sa \in S_j^{in} \\ \rho_{in}(s,sa)}} mu(sa,j,p-1) = \sum_{\substack{sa \in S_j^{out} \\ \rho_{out}(s,sa)}} mp(sa,j,p), \quad \forall \; j \in J, s \in S_j^{eff}, p \in P, p > 1 \qquad (A3)$$

$$mu(sa,j,p-1) = Stoi1 * mp(sb,j,p), \quad \forall \; j \in J, sa \in S_j^{in}, sb \in S_j^{out}, p \in P, p > 1 \qquad (A4)$$

$$mu(sa,j,p) = Stoi2 * mu(sb,j,p), \quad \forall \; j \in J, sa, sb \in S_j^{in}, p \in P \qquad (A5)$$

$$qs(s,p) = q_s^o - \sum_{j \in S_j^{in}} mu(s,j,p), \quad \forall \; s \notin S^p, p \in P, p = 1 \qquad (A6)$$

$$qs(s,p) = q_s^o - d(s,p), \quad \forall \; s \in S^p, p \in P, p = 1 \qquad (A7)$$

$$qs(s,p) = qs(s,p-1) - \sum_{j \in S_j^{in}} mu(s,j,p), \quad \forall \; s \in S^f, p \in P, p > 1 \qquad (A8)$$

$$qs(s,p) = qs(s,p-1) - \sum_{j \in S_j^{in}} mu(s,j,p) + \sum_{j \in S_j^{out}} mp(s,j,p),$$

$$\forall \; s \notin S^f, S^P, p \in P, p > 1 \qquad (A9)$$

$$qs(s,p) = qs(s,p-1) + \sum_{j \in S_j^{out}} mp(s,j,p) - d(s,p), \quad \forall \; s \in S^p, p \in P, p > 1 \qquad (A10)$$

Duration Constraints:

$T_p(sa,j,p) = T_u(s,j,p-1) + \alpha_j^s \, y(s,j,p-1),$

$\forall \ j \in J, s \in S_j^{eff}, sa \in S_j^{out}, \rho_{out}(s,sa), p \in P, p > 1 \qquad (A11)$

$$T_u(s,j,p) \geq \sum_{\substack{\rho 1 \in P \\ 1 \leq p1 \leq p}} \sum_{\substack{sa \in S_j^{eff} \\ \rho_{out(sa,sb)}}} \sum_{sb \in S_j^{out}} \Big(T_p(sb,j,p1) - T_u(sa,j,p1-1)\Big),$$

$\forall \ j \in J, s \in S_j^{eff}, p \in P, p > 1 \qquad (A12)$

Sequence Constraints:

$T_u(s,j,p) \geq T_p(sa,j,p), \quad \forall \ j \in J, s \in S_j^{eff}, sa \in S_j^{out}, p \in P \qquad (A13)$

$T_u(s,j,p) \geq T_p(s,j1,p), \quad \forall \ j, j1 \in J, s \in S_j^{in}, S_{j1}^{out}, j \neq j1, p \in P \qquad (A14)$

$T_u(s,j,p) \leq H, \quad \forall \ j \in J, s \in S_j^{in}, p \in P \qquad (A15)$

$T_p(s,j,p) \leq H, \quad \forall \ j \in J, s \in S_j^{out}, p \in P \qquad (A16)$

$T_u(s,j,p) = T_u(sa,j,p), \quad \forall \ j \in J, s, sa \in \rho_{in}(s,sa), p \in P \qquad (A17)$

$qs(s,p) \leq q_s^{max}, \quad \forall \ s \notin S^f, S^p, p \in P \qquad (A18)$

Direct and Indirect Heat integration constraints:

$$\sum_{j1 \in J_c} \sum_{\substack{sa \in S_j^c, S_{j1}^{in} \\ temp_{j1}^{sa}}} X(s,j,sa,j1,p) \leq y(s,j,p), \ \forall \ j \in J_h, s \in S_j^h, S_j^{in}, Temp_j^s, p \in P \qquad (A19)$$

$$\sum_{j \in J_h} \sum_{\substack{s \in S_j^h, S_j^{in} \\ temp_j^s}} X(s,j,sa,j1,p) \leq y(sa,j1,p), \forall \ j1 \in J_c, sa \in S_j^c, S_{j1}^{in}, Temp_{j1}^{sa}, p \in P \qquad (A20)$$

$$\sum_{j \in J_h} \sum_{\substack{s \in S_j^h, S_j^{in} \\ temp_j^s}} Z(s,j,u,p) + \sum_{j1 \in J_c} \sum_{\substack{sa \in S_j^c, S_{j1}^{in}, \\ temp_{j1}^{sa}}} z(sa,j1,u,p) \leq 1, \quad \forall \quad p \in P, u \in U \qquad (A21)$$

$$\sum_{j1\in J_c}\sum_{\substack{sa\in S_j^c,S_{j1}^{in}\\ temp_{j1}^{sa}}} X(s,j,sa,j1,p)+z(s,j,u,p)\le 1,$$

$$\forall\ \ j\in J_h, s\in S_j^h, S_j^{in}, Temp_j^s\ , u\in U, p\in P \tag{A22}$$

$$\sum_{j\in J_h}\sum_{\substack{s\in S_j^h,S_j^{in}\\ temp_j^s}} X(s,j,sa,j1,p)+z(sa,j1,u,p)\le 1,$$

$$\forall\ \ j1\in J_c, sa\in S_j^c, S_{j1}^{in}, Temp_{j1}^{sa}\ , u\in U, p\in P \tag{A23}$$

$$qes(s,j,u,p-1)=wt(u)\,c_p^f(u)\left(T^o(u,p-1)-T^f(u,p)\right)z(s,j,u,p-1),$$

$$\forall\ \ j\in J_h, s\in S_j^h, S_j^{in}, Temp_j^s\ , u\in U, p\in P, p>1 \tag{A24}$$

$$qes(sa,j1,u,p-1)=wt(u)\,c_p^f(u)\left(T^f(u,p)-T^o(u,p-1)\right)z(sa,j1,u,p-1),$$

$$\forall\ \ j1\in J_c, sa\in S_j^c, S_{j1}^{in}, Temp_{j1}^{sa}\ , u\in U, p\in P, p>1 \tag{A25}$$

$$T^o(u,p)=T^f(u,p),\quad \forall\ \ u\in U, p\in P, p>1 \tag{A26}$$

$$T^o(u,p-1)\le T^f(u,p)+T_j\left(\sum_{j\in J_h}\sum_{\substack{s\in S_j^h,S_j^{in}\\ temp_j^s}} z(s,j,u,p-1)\right.$$

$$\left.+\sum_{j1\in J_c}\sum_{\substack{sa\in S_j^c,S_{j1}^{in}\\ temp_{j1}^{sa}}} z(sa,j1,u,p-1)\right),\quad \forall\quad u\in U, p\in P, p>1 \tag{A27}$$

$$T^o(u,p-1)\ge T^f(u,p)-T_j\left(\sum_{j\in J_h}\sum_{\substack{s\in S_j^h,S_j^{in}\\ temp_j^s}} z(s,j,u,p-1)\right.$$

$$\left.+\sum_{j1\in J_c}\sum_{\substack{sa\in S_j^c,S_{j1}^{in}\\ temp_{j1}^{sa}}} z(sa,j1,u,p-1)\right),\ \forall\quad u\in U, p\in P, p>1 \tag{A28}$$

$$Temp_{j1}^{sa}-Temp_j^s\ge \Delta T^{min}-T_j\left(1-x(s,j,sa,j1,p-1)\right),$$

$$\forall \;\; j \in J_h, s \in S_j^h, S_j^{in}, Temp_j^s \;, j1 \in J_c, sa \in S_j^c, S_{j1}^{in}, Temp_{j1}^{sa}, p \in P, p > 1 \qquad (A29)$$

$$T^f(u,p) - Temp_j^s \; \geq \Delta T^{min} - T_j\big(1 - z(s,j,u,p-1)\big),$$
$$\forall \;\; j \in J_h, s \in S_j^h, S_j^{in}, Temp_j^s \;, p \in P, p > 1 \qquad (A30)$$

$$Temp_{j1}^{sa} - T^f(u,p) \geq \Delta T^{min} - T_j\big(1 - z(sa,j1,u,p-1)\big),$$
$$\forall \;\; j1 \in J_c, sa \in S_j^c, S_{j1}^{in}, Temp_{j1}^{sa} \;, u \in U, p \in P, p > 1 \qquad (A31)$$

$$E_j^s \; y(s,j,p) = qes(s,j,u,p) + st(s,j,p) + \sum_{j1 \in J_c} \sum_{\substack{sa \in S_j^c, S_{j1}^{in}, \\ temp_{j1}^{sa}}} x(s,j,sa,j1,p) E_{j1}^{sa} \;,$$

$$\forall \;\; j \in J_h, s \in S_j^h, S_j^{in}, Temp_j^s \;, u \in U, p \in P \qquad (A32)$$

$$E_{j1}^{sa} \; y(sa,j1,p) = qes(sa,j1,u,p) + st(sa,j1,p) + \sum_{j \in J_h} \sum_{\substack{s \in S_j^h, S_j^{in}, \\ temp_j^s}} x(s,j,sa,j1,p) E_{j1}^{sa} \;,$$
$$\forall \;\; j1 \in J_c, sa \in S_j^c, S_{j1}^{in}, Temp_{j1}^{sa} \;, u \in U, p \in P \qquad (A33)$$

$$T_p(s,j,p) \geq T_p(sa,j1,p) - M\big(1 - x(s,j,sa,j1,p-1)\big),$$

$$\forall \;\; j \in J_h, s \in S_j^h, S_j^{in}, Temp_j^s \;, j1 \in J_c, sa \in S_j^c, S_{j1}^{in}, Temp_{j1}^{sa}, p \in P, p > 1 \qquad (A34)$$

$$T_p(s,j,p) \leq T_p(sa,j1,p) + M\big(1 - x(s,j,sa,j1,p-1)\big),$$
$$\forall \;\; j \in J_h, s \in S_j^h, S_j^{in}, Temp_j^s \;, j1 \in J_c, sa \in S_j^c, S_{j1}^{in}, Temp_{j1}^{sa}, p \in P, p > 1 \qquad (A35)$$

$$T_u(s,j,p) \geq utu(s,j,u,p) - M\big(y(s,j,p) - z(s,j,u,p)\big),$$

$$\forall \;\; j \in J_h, J_c, s \in S_j^{in}, Temp_j^s, u \in \; U, p \in P \qquad (A36)$$

$$T_u(s,j,p) \leq utu(s,j,u,p) + M\big(y(s,j,p) - z(s,j,u,p)\big),$$
$$\forall \;\; j \in J_h, J_c, s \in S_j^{in}, Temp_j^s, u \in \; U, p \in P \qquad (A37)$$

$$utp(s,j,u,p) \geq T_u(s,j,p-1) + \alpha_j^s\big(y(s,j,p-1)\big) - M \;\; (y(s,j,p-1) -$$
$$z(s,j,u,p-1)), \qquad \forall \;\; j \in J_h, J_c, s \in S_j^{in}, Temp_j^s, u \in \; U, p \in P, p > 1 \qquad (A38)$$

$$utp(s,j,u,p) \leq T_u(s,j,p-1) + \alpha_j^s\big(y(s,j,p-1)\big) + M \;\; (y(s,j,p-1) -$$
$$z(s,j,u,p-1)), \qquad \forall \;\; j \in J_h, J_c, s \in S_j^{in}, Temp_j^s, u \in \; U, p \in P, p > 1 \qquad (A39)$$

$utu(s,j,u,p) \geq utp(s,j,u,p),$

$$\forall \;\; j \in J_h, J_c, s \in S_j^{in}, Temp_j^s, u \in \; U, p \in P \qquad (A40)$$

$utu(s,j,u,p) \geq utp(sa,j1,u,p),$

$$\forall \;\; j \in J_h, J_c \;, j1 \in J_h, J_c \;, j \neq j1, s \in S_j^{in}, Temp_j^s, sa \in S_{j1}^{in}, Temp_{j1}^{sa}, u \in \; U, p \in P \qquad (A41)$$

$$Profit\; Z = \sum_{s \in S^p} \sum_{p \in P} d\,(s,p) * price(s) - \sum_{j \in up_j^s} \sum_{\substack{s \in S_j^{in}, E_j^s \\ s_j^{eff}}} \sum_{p \in P} st(s,j,p) up_j^s \qquad (A42)$$

Nomenclature

Indices

s	State
$j, j1$	Units
p	Time point
u	Heat storage vessel

Sets

J	Set of units
S	Material states
S_j^{in}	Input states to unit *j*
S_j^{out}	Input states to unit *j*
S_j^{eff}	Effective state for unit *j*
J_c	Unit handling a task require cooling
J_h	Unit handling a task require heating
S_J^C	Input state to unit *j* which is handling task require cooling
S_J^h	Input state to unit *j* which is handling task require heating
P	Time points within the time horizon
U	Heat storage units
S^P	Product states
S^F	Feed states

Parameters

q_s^o	Initial amount of material available for state *s*
q_s^{max}	Maximum storage capacity for state *s*
P_s	Price of state of product state s ϵ S^P
H	Scheduling time horizon
M	Large positive numbers in big-M constraints
V_j	Maximum processing capacity of unit *j*
α_j^s	Constant batch processing time of input state *s* ϵ S_j^{eff} in unit *j*
E_j^s	Amount of heat required by or removed from unit *j* conducting the task
Up_j^s	Price of external utility required by unit *j* conducting the task corresponding to state s ϵ S_j^{in}
$Temp_j^s$	Operating temperature of processing unit *j* conducting the task corresponding to state s ϵ S_j^{eff}
$\rho_{in}(s,sa)$	Other input states sa ϵ S_j^{in} to the task corresponding to a state s ϵ S_j^{eff}
$\rho_{out}(s,sa)$	Output states sa ϵ S_j^{out} to the task corresponding to a state s ϵ S_j^{eff}
ΔT^{min}	Minimum temperature difference
$T^{uu}(u)$	Upper temperature of utility
$T^{lu}(u)$	Lower temperature of utility
$C_p^f(u)$	Heat capacity of heat storage fluid
$W^l(u)$	Lower bound of storage capacity in terms of storage fluid amount
$W^u(u)$	Upper bound of storage capacity in terms of storage fluid amount

Binary variables

$y(s,j,p)$	Binary variable corresponding to the utilization of state s ϵ S_j^{eff} by unit *j* at the time point *p*
$x(s,j,sa,j1,p)$	Binary variable associated with heat integration between the unit *j* ϵ J_h performing the task corresponding to state *s* ϵS and the unit *j*1ϵJc performing the task corresponding to state *s* ϵsa at time point *p*
$z(s,j,u,p)$	Binary variable for heat exchange between the unit *j* performing the task corresponding to state *s* ϵS and heat storage vessel u at time point *p*

Positive variables

$T_p(s,j,p)$	Time at which state *s* ϵ S_j^{out} is produced at time point *p*

$T_u(s,j,p)$	Time at which state $s \in S_j^{in}$ is used at time point p
$qs(s,p)$	Amount of state s stored at time point p
$m_p(s,j,p)$	Amount of state $s \in S_j^{out}$ is produced at time point p
$m_u(s,j,p)$	Amount of state $s \in S^P$ delivered to customers at time point p
$cw(s,j,p)$	Cold utility requirement for the unit $j \in J_c$ performing the task corresponding to state $s \in S_j^{eff}$ at time point p
$st(s,j,p)$	Hot utility requirement for the unit $j \in J_h$ performing the task corresponding to state $s \in S_j^{eff}$ at time point
$qes(s,j,u,p)$	Amount of heat exchange between storage unit u and unit $j \in (J_c \cup J_h)$ performing the task corresponding to state $s \in S_j^{eff}$ at time point p
$T^o(u,p)$	Initial temp in storage unit u at time point p
$T^f(u,p)$	Final temp in storage unit u at time point p
$utu(s,j,u,p)$	Time at which heat storage unit commences activity by integrating with unit $j \in (J_c \cup J_h)$ performing the task corresponding to state $s \in S_j^{eff}$ at time point p
$utp(s,j,u,p)$	Time at which heat storage unit ends activity after exchanging heat with unit $j \in (J_c \cup J_h)$ performing the task corresponding to state $s \in S_j^{eff}$ at time point p
$wt(u)$	Capacity of heat storage unit u

Appendix B

B1: Nomenclature for scheduling and direct heat Integration model presented in Chapter 3

Indices

$n1, n2, n3$	Events
$i, i1$	Tasks
$j, j1$	Units
s	State

Sets

I	Set of tasks
J	Set of units
I_j	Set of tasks that can be performed in unit *j*
I_s^c	Tasks which consume state *s*
I_s^p	Tasks which produce state *s*
I_c	Task which requires cooling
I_h	Task which requires heating
N	Event points within the time horizon
U	Utilities
S	States
S^{IN}	States that are intermediates
S^R	States that are raw materials
S^P	States that are final products
S^{dfis}	Intermediate states with dedicated finite intermediate storage (dfis)

Parameters

B_i^{max}	Maximum batch size of task *i*
B_i^{min}	Minimum batch size of task *i*
Δn	Limit on the maximum number of events over which a task is allowed to continue
$price_s$	Price of product state *s*
M	Large positive numbers in big-M constraints
ρ_{is}	Fraction of state *s* produced $(\rho_{is} \geq 0)$ by task *i* Fraction of state *s* consumed$(\rho_{is} \leq 0)$ by task *i*

δ_i	Coefficient of variable term of processing time of task *i*
γ_i	Coefficient of constant term of processing time of task *i*
ST_s^{max}	Maximum amount of state *s*
ST_s^o	Initial amount available for state *s*
H	Short-term time horizon
c_{uc}	Unit cost of cooling utility *u* over interval *t*
c_{uh}	Unit cost of heating utility *u* over interval *t*
α_i', α_{i1}'	Coefficient of constant terms of external utility requirements of task *i* when operated in a with heat integration mode.
α_i, α_{i1}	Coefficient of constant terms of external utility requirements of task *i* when operated in a without heat integration mode.
β_i', β_{i1}'	Coefficient of variable terms of external utility requirements of task *i* when operated in a with heat integration mode.
β_i, β_{i1}	Coefficient of variable terms of external utility requirements of task *i* when operated in a without heat integration mode.

Binary variable

$x(i, i1, n1)$	Binary variable associated with heat integration of task *i* and *i1* at event *n1*
$w(i, n1, n2)$	Binary variable that assign of the task *i* that starts at event *n1* and ends at event *n2*

Positive variable

$b(i, n1, n2)$	Amount of material processing by task *i* starting at event *n1* and ends at event *n2*
$T^S(i, n1)$	Starting time of a task *i* at event *n*1
$T^f(i, n1)$	Finishing time of a task *i* at event *n*1
$ST_o(s)$	Initial amount of state *s* required from external resources
$ST(s, n1)$	Excess amount of state *s* that needs to be stored at event *n1*
$q(i, n1)$	Amount of heating utility required by task *i* when operating in a standalone mode
$q1(i, n1)$	Amount of heating utility required by task *i* when operating in a heat-integrated mode
$q(i1, n1)$	Amount of cooling utility required by task *i1* when operating in a

	standalone mode
$q1(i1, n1)$	Amount of cooling utility required by task *i1* when operating in a heat-integrated mode
$bh(i, i1, n1)$	Amount of batch processed by heat-integrated tasks *i* which require Heating
$bc(i, i1, n1)$	Amount of batch processed by heat-integrated tasks *i* which require Cooling

B2: Nomenclature for heat integration and cyclic scheduling model presented in Chapter 4

Indices

$i, i1$	Tasks
$j, j1$	Units
s	State
u	Utilities
$n1, n2, n3, n^a, n^b$	Events

Sets

I	Set of tasks
J	Set of units
I_j	Set of tasks that can be performed in unit *j*
I_s^c	Tasks which consume state *s*
I_s^p	Tasks which produce state *s*
N	Event points within the time horizon
U	Utilities
S	States
S^{IN}	States that are intermediates
S^R	States that are raw materials
S^P	States that are final products
S^{dfis}	Intermediate states with dedicated finite intermediate storage (dfis)

Parameters

B_i^{max}	Maximum batch size of task *i*

B_i^{min}	Minimum batch size of task *i*
Δn	Limit on the maximum number of events over which a task is allowed to continue
$price_s$	Price of product state *s*
M	Large positive numbers in big-M constraints
ρ_{is}	Fraction of state *s* produced $(\rho_{is} \geq 0)$ by task *i*
	Fraction of state *s* consumed$(\rho_{is} \leq 0)$ by task *i*
δ_i	Coefficient of variable term of processing time of task *i*
γ_i	Coefficient of constant term of processing time of task *i*
ST_s^{max}	Maximum amount of state *s*
ST_s^{o}	Initial amount available for state *s*
H	Short-term time horizon
c_{uc}	Unit cost of cooling utility *u* over interval *t*
c_{uh}	Unit cost of heating utility *u* over interval *t*
α_i', α_{i1}'	Coefficient of constant terms of external utility requirements of task *i* when operated in a with heat integration mode.
α_i, α_{i1}	Coefficient of constant terms of external utility requirements of task *i* when operated in a standalone mode.
β_i', β_{i1}'	Coefficient of variable terms of external utility requirements of task *i* when operated in a with heat integration mode.
β_i, β_{i1}	Coefficient of variable terms of external utility requirements of task *i* when operated in a standalone mode.
γ_i, γ_{i1}	Coefficient of constant terms of processing time of task *i* when operated in a standalone mode.
γ_i', γ_{i1}'	Coefficient of variable terms of external utility requirements of task *i* when operated in a with heat integration mode.

Binary variable

$x(i, i1, n1)$	Binary variable associated with heat integration of task *i* and *i1* at event *n1*
$w(i, n1, n2)$	Binary variable that represents of the task *i* that starts at event *n1* and ends at event *n2*

Positive variable

$b(i, n1, n2)$	Amount of material processing by task *i* starting at event *n1* and ends at event *n2*
$T^S(i, n1)$	Starting time of a task *i* at event $n1$
$T^f(i, n1)$	Finishing time of a task *i* at event $n1$
$ST_o(s)$	Initial amount of state *s* required from external resources
$ST(s, n1)$	Excess amount of state *s* that needs to be stored at event *n1*
$q(i, n1)$	Amount of heating utility required by task *i* when operating in a standalone mode
$q1(i, n1)$	Amount of heating utility required by task *i* when operating in a heat-integrated mode
$q(i1, n1)$	Amount of cooling utility required by task *i1* when operating in a standalone mode
$q1(i1, n1)$	Amount of cooling utility required by task *i1* when operating in a heat-integrated mode
$bh(i, i1, n1)$	Amount of material processed by heat-integrated tasks *i* which require Heating
$bc(i, i1, n1)$	Amount of material processed by heat-integrated tasks *i* which require Cooling

B3: Nomenclature for short term scheduling and heat integration of batch plants: Design and optimization of heat storage vessels presented in Chapter 5

Abbreviations

cu	Relative cost units
$USEB$	Unit Specific Event Based

Indices

$n, n', n1, n2, n3$	Events
$i, i', i1$	Tasks
$j, j1$	Units
u	Heat storage unit
s	State

Sets

I	Set of tasks
J	Set of units
I_j	Set of tasks that can be performed in unit *j*
I_s^c	Tasks consume state *s*
I_s^p	Tasks produce state *s*
N	Event points within the time horizon
I_c	Tasks require cooling
I_h	Tasks require heating
U	Heat storage units
S	Material states
S^{IN}	Intermediate material states
S^R	Raw materials
S^P	Final products
S^{dfis}	Intermediate states with dedicated finite intermediate storage (dfis)

Parameters

B_i^{max}	Maximum batch size of task *i*
B_i^{min}	Minimum batch size of task *i*
Δn	Maximum number of events over which a task is allowed to continue
$price_s$	Price of product state *s*
M, MM	Large positive numbers in big-M constraints
ρ_{is}	Fraction of state *s* produced $(\rho_{is} \geq 0)$ or consumed$(\rho_{is} \leq 0)$ by task *i*
δ_i	Coefficient of variable term of task *i* processing time
γ_i	Coefficient of constant term of task *i* processing time
ST_s^o	Initial amount available for state *s*
H	Short-term time horizon
c_c	Unit cost of cooling utility
c_h	Unit cost of heating utility
$qmt(i)$	Amount of energy released or required by task *i*
$C_p(u)$	Heat capacity of heat storage medium
$C_p(i)$	Heat capacity of processing task *i*
$wt(u)$	Mass flow rate of heat storage medium

ΔT_{min}	Minimum temperature approach
$T^u(u)$	Maximum temperature of storage medium *u*
$T^l(u)$	Minimum temperature of storage medium *u*
$T_j(i)$	Operating temperature of task *i*
$T^{pi}(i)$	Inlet temperature of processing task *i*
$T^{po}(i)$	Outlet temperature of process task *i*
$W^u(u)$	Maximum flow rate of storage medium *u*
$W^l(u)$	Minimum flow rate of storage medium *u*
A_f	Annualizing factor
θ	Cost function exponent
C_{cost}	Fixed cost of heat storage vessel
V_{cost}	Variable cost of heat storage vessel
a	Annual fractional interest rate
LSV	Life span of storage vessel

Binary variable

$x(i,i',n)$	1 if task *i* and *i'* are heat integrated at event *n*
	0 otherwise
$w(i,n1,n2)$	1 if task *i* starts at event *n*1 and ends at event *n*2
	0 otherwise
$hex(i,u,n)$	1 if task *i* and heat storage medium *u* are heat integrated at event *n*
	0 otherwise
$ns(u)$	1 if the storage tank is utilized
	0 otherwise

Positive variable

$b(i,n1,n2)$	Batch amount processing by task *i* starting at event *n*1 and ending at event *n*2
$T^S(i,n1)$	Starting time of a task *i* at event *n*1
$T^f(i,n1)$	Finishing time of a task *i* at event *n*1
$ST_o(s)$	Initial amount of state *s* required from external resources
$ST(s,n1)$	Amount of material state *s* stored at event *n*1
$q(i,n1)$	Amount of external utility required by task *i*
$qs(i,u,n1)$	Amount of heat exchanged between task *i* and storage medium *u* at

	event *n*1
$TT^s(u,n1)$	Initial temperature of storage medium *u* at event *n*1
$TT^f(u,n1)$	Final temperature of storage medium *u* at event *n*2
$HT^s(u,n1)$	Starting time of a heat storage task at event *n*1
$HT^f(u,n1)$	Finishing time of a heat storage task at event *n*1
$vqmt(i,n)$	Amount of energy released or required by task *i* at event *n*
$mqmt(i,ii,n)$	Amount of energy exchanged during the direct integration at event *n*

Appendix B4: Nomenclature for Long term scheduling and heat integration of batch plants: Direct and indirect heat transfer using storage vessels presented in Chapter 6

Indices

$i, i1$	Tasks
$j, j1$	Units
s	State
u	Utilities
$n1, n2, n^a, n^b$	Events

Sets

I	Set of tasks
J	Set of units
I_j	Set of tasks that can be performed in unit *j*
I_s^c	Tasks which consume state *s*
I_s^p	Tasks which produce state *s*
N	Event points within the time horizon
U	Utilities
S	States
S^{IN}	States that are intermediates
S^R	States that are raw materials
S^P	States that are final products
S^{dfis}	Intermediate states with dedicated finite intermediate storage (dfis)

Parameters

B_i^{max}	Maximum batch size of task *i*
B_i^{min}	Minimum batch size of task *i*
Δn	Maximum number of events over which a task is allowed to continue
$price_s$	Price of product state *s*
M	Large positive numbers in big-M constraints
ρ_{is}	Fraction of state *s* produced $(\rho_{is} \geq 0)$ by task *i*
H	Short-term time horizon
$qmt(i)$	Amount of energy released or required by task *i*
$C_p(u)$	Heat capacity of heat storage medium
$C_p(i)$	Heat capacity of processing task *i*
$wt(u)$	Mass flow rate of heat storage medium
$eqlcu(u)$	The amount of external cold utility required to cool
$eqlhu(u)$	The amount of external hot utility required to heat

Binary variable

$x(i, i1, n1)$	1 if task *i* and *i1* are heat integrated at event *n1*
	0 otherwise
$w(i, n1, n2)$	1 if task *i* starts at event *n*1 and ends at event *n*2
	0 otherwise
$hex(i, u, n)$	1 if task *i* and heat storage medium *u* are heat integrated at event *n*
	0 otherwise

Positive variable

$b(i, n1, n2)$	Batch amount processing by task *i* starting at event *n*1 and ending at event *n*2
$T^S(i, n1)$	Starting time of a task *i* at event *n*1
$T^f(i, n1)$	Finishing time of a task *i* at event *n*1
$ST(s, n1)$	Excess amount of state *s* that needs to be stored at event *n1*
$q(i, n1)$	Amount of heating utility required by task i when operating in a standalone mode
$qhi(i, n1)$	Amount of heating utility required by task *i* when operating in a heat-integrated mode
$TT^s(u, n1)$	Initial temperature of storage medium *u* at event *n*1
$TT^f(u, n1)$	Final temperature of storage medium *u* at event *n*2

$HT^s(u,n1)$	Starting time of a heat storage task at event $n1$
$HT^f(u,n1)$	Finishing time of a heat storage task at event $n1$
$mqmt(i,ii,n)$	Amount of energy exchanged during the direct integration at event n

Publications in Present Work

Journals

1. Mummana, S. S., Seepana, M. M., & Vooradi, R. (2020). "Simultaneous scheduling and heat integration of batch plants using unit-specific event based modelling". *Chemical Product and Process Modeling*, 2. https://doi.org/10.1515/cppm-2019-0070.
2. Mummana, S. S., Vooradi, R. (2020). "Heat integration and cyclic scheduling of multipurpose batch plants using three index unit-specific event based model". *Chemical Engineering Communications*, 1-22. https://doi.org/10.1080 /00986445.2020.1765160.
3. Mummana, S. S., Anne, S. B., & Vooradi, R. (2021). A simple unit specific event based modeling framework for short term scheduling and heat integration of batch plants: Design and optimization of heat storage vessels. *Computers & Chemical Engineering*, *145*, 107155. https://doi.org/10.1016 /j.comp chemeng.2020.107155.

Conference Presentations

1. Mummana, S. S., Seepana, M. M., & Vooradi, R. (2018). "Direct heat integration of multipurpose batch plants using three index unit specific event based model" ICEE 2018, 9-10 March, 2018 at NIT Calicut.
2. Mummana, S. S., Vooradi, R. (2019). "Unit specific event based model for short-term scheduling of multipurpose batch plants with heat integration" INCEEE 2019, 15 - 16 February, 2019 at NIT Warangal.