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OPTIMUM HEAT STORAGE DESIGN FOR HEAT INTEGRATED MULTIPURPOSE BATCH PLANTS

by

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Synopsis

The application of heat integration to minimise energy usage in multipurpose batch plants has been in published literature for more than two decades. Direct heat integration may be exploited when the heat source and heat sink processes are active over a common time interval. Alternately, indirect heat integration involves using a heat transfer fluid for storing energy and allows heat integration of processes regardless of the time interval. This is possible as long as the heat source process takes place before the heat sink process. This allows heat to be stored and then used later when required. In both cases, heat transfer may only take place if the thermal driving forces allow. For most present methods, the schedule tends to be fixed and as such, time is also fixed *a priori*, which leads to suboptimal results. The method presented in this dissertation treats time as a variable and consequently leads to improved results. Both direct and indirect heat integration are considered as well as the optimisation of the heat storage size and the initial temperature of the heat storage fluid. The mathematical formulation is based on an uneven discretisation of the time horizon and the state sequence network (SSN) recipe representation, which has proven to result in mathematical models with fewer binary variables compared to models based on other representations (Majozi & Zhu, 2001). The resulting model exhibits the mixed integer nonlinear programming (MINLP) structure, which implies that global optimality cannot generally be guaranteed. However, a procedure is presented that seeks to find a globally optimal solution, even for nonlinear problems. Heat losses from the heat storage vessel are also considered. This work is an extension of the MILP model of Majozi (2009), which was in fact more suited to multiproduct rather than multipurpose batch facilities. The addition of heat storage instead of using only direct heat integration leads to increased flexibility in the process and therefore improved energy usage. Optimising the size of the heat storage vessel as well as the initial temperature of the heat storage fluid decreased the requirement for external hot utility for an industrial case study by 33% compared to using known parameters.

Declaration

I, Jane Dorothy Stamp, student number 24035069, declare that:

1. I understand what plagiarism is and am aware of the University's policy in this regard.
2. I declare that this dissertation is my own original work. Where other people's work has been used (either from a printed source, internet or any other source), this has been properly acknowledged and referenced in accordance with departmental requirements.
3. I have not used work previously produced by another student or any other person to hand in as my own.
4. I have not allowed and will not allow anyone to copy my work with the intention of passing it off as his or her own work.
5. The work presented in this dissertation has not been submitted anywhere else in partial or full fulfillment of another degree.

Student________________

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CHAPTER 1

INTRODUCTION

1.1 Background

Process integration may be defined as “a holistic approach to process design, retrofitting and operation which emphasizes the unity of the process” (El-Halwagi, 1997: 3). The objective of process integration is to optimise the use of resources, energy and equipment and can have a significant effect on the efficiency and revenue of a plant. This dissertation considers the design of a heat storage vessel for heat integrated multipurpose batch plants.

A batch process is a series of independently operated tasks, which allows improved control in terms of quality and yield compared to continuous processes (Pourali *et al.*, 2006). Batch processes are commonly used for the manufacture of products required in small quantities or for specialty and complex products of high value. Approximately half of all production facilities make use of batch processes (Stoltze *et al.*, 1995). Batch plants are also popular due to their flexible and adaptable nature, which is particularly important in volatile markets.

Batch operations are generally run on a smaller scale compared to continuous operations and utility requirements have in the past been considered less significant. Heat integration in batch plants has therefore largely been ignored. However, utility requirements in some batch plants, such as in the food industry, breweries, dairies, meat processing facilities, biochemical plants and agrochemical facilities, contribute largely to their overall cost.

Pinch analysis, originally developed for heat integration in continuous processes, has been modified for batch plants. However, hot and cold streams in batch plants are not continuously available. Methods usually depend on a predefined schedule, where energy requirements are averaged over time intervals (Kemp, 1990). This, however, leads to suboptimal results. Methods which capture the essence of time and are specifically applicable to batch plants are therefore required.

Heat integration may be achieved in two ways in a batch process. If the operating schedule allows an overlap in time of hot and cold units, direct heat integration may be used with both units required to be active. However, due to the time dependent nature of batch processes it may be necessary to store heat from a hot unit using an intermediate heat storage fluid and reuse this heat at a later time where it is required, resulting in indirect heat integration. The design of the heat storage vessel can then be optimised in terms of capacity as well as initial temperature to improve opportunities for indirect heat integration. Heat losses from the heat storage vessel must also be considered as these reduce the efficiency of the heat storage system. These aspects are addressed in this investigation.

1.2 Problem statement and objectives

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

Given:

(i) Production scheduling data, including equipment capacities, durations of tasks, time horizon of interest, product recipes, cost of starting materials and selling price of final products,

(ii) Hot duties for tasks requiring heating and cold duties for tasks that require cooling,

(iii) Cost of hot and cold utilities,

(iv) Operating temperatures of heat sources and heat sinks,

(v) Minimum allowable temperature differences, and

(vi) Design limits on heat storage,

Determine:

(i) An optimal production schedule where the objective is to maximise profit, defined as the difference between revenue and the cost of hot and cold utilities.

(ii) The optimal size of heat storage available as well as the initial temperature of heat storage.

The proposed method also takes into account heat losses from the heat storage vessel during times when it is idle.

1.3 Scope

Time was treated as a variable rather than allowing the schedule to be predefined. Mathematical modelling based on the state sequence network (SSN) recipe representation (Majozi and Zhu, 2001) resulted in a mixed integer nonlinear programming (MINLP) formulation. The model for simultaneous short-term scheduling and heat integration in multipurpose batch plants was developed and applied to various problems of industrial relevance. In all cases, batch sizes and processing times were fixed. The heat storage capacity and initial storage temperature were optimised. Heat losses from the heat storage vessel during idle times were investigated. The proposed method was limited to short-term scheduling due to the structure of the mixed integer mathematical problem. As the time horizon increases, the number of binary variables increases, which leads to larger problems with longer solution times.

1.4 Structure

The rest of this dissertation contains the literature review concerning short-term scheduling and heat integration in Chapter 2. Thereafter, the mathematical model is developed in Chapter 3 with results from its application to selected examples in Chapter 4. Conclusions are then presented in Chapter 5. References follow each chapter.

1.5 References

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CHAPTER 2

LITERATURE REVIEW

2.1 Introduction

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

The main focus of this chapter, however, is incorporating heat integration into batch plant scheduling. Both direct and indirect heat integration strategies are discussed. Examples are also given of how heat integration has been applied to energy intensive batch processes. The complete heat integration formulation based on the state sequence network (SSN) is given, as this forms the basis for the current work. This model optimises both the processing schedule and heat integration simultaneously and requires fewer binary variables compared to other models. Heat integration in continuous processes has not been included as this is well understood and is covered extensively in published literature.

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

2.2 Operation of batch plants

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

2.3 Operational philosophies

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

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

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

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

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

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

MIS: Mixed Intermediate Storage. This combines the use of UIS, NIS, FIS and ZW.

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

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

2.4 Scheduling in batch processes

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

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

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

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

2.5 Time horizon representation

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

2.5.1 Uniformly discretised time horizon

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

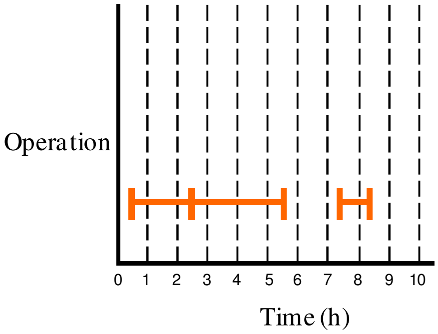

Figure 2.1. Tasks are not accurately represented.

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

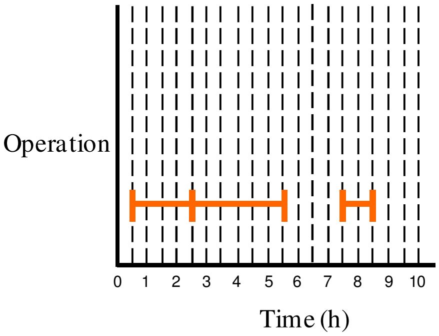

Figure 2.2. Tasks represented accurately, many unnecessary intervals.

2.5.2 Uneven discretisation of the time horizon

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

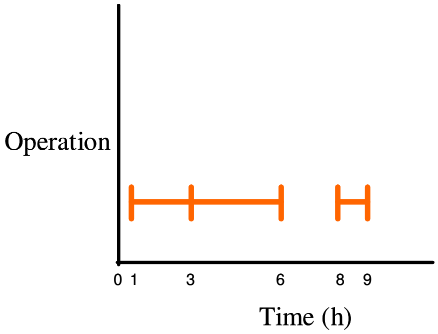

Figure 2.3. Uneven discretisation of the time horizon.

A drawback of the uneven discretisation of the time horizon is that the number of time points must be determined iteratively (Ierapetritou & Floudas, 1998; Shaik & Floudas, 2009).

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

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

2.6 Flowsheet representation

The flowsheet is generally represented by the State Task Network (STN), Resource Task Network (RTN) or more recently the State Sequence Network (SSN).

2.6.1 State Task Network (STN)

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

2.6.2 Resource Task Network (RTN)

The RTN was proposed by Pantelides (1994). The overall production facility is modelled as a collection of tasks and resources with some of the resources consumed and others formed. The resources include feeds, intermediates, products, energy, manpower, storage and transportation facilities. The tasks are defined as for the STN, but also include transportation, cleaning and storage. An advantage of the RTN over the STN arises in problems involving identical equipment. Here the RTN formulation introduces a single binary variable instead of the multiple variables as used by the STN (Mendez *et al.*, 2006).

2.6.3 State Sequence Network (SSN)

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

2.7 Early mathematical methods for scheduling

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

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

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

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

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

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

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

2.8 Short-term scheduling methods based on the STN

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

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

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

2.9 Short-term scheduling methods based on the RTN

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

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

A similar procedure based on the RTN representation was proposed by Schilling and Pantelides (1996). They used time points and time slots to represent the beginning and ending of tasks. Nonlinearities from the duration and resource balance constraints yielded a

MINLP. These nonlinearities were linearised using the Glover transformation (Glover, 1975) and the resultant formulation was a MILP. Due to a large integrality gap as seen with formulations using an uneven discretisation of the time horizon, a novel branch and bound algorithm was used rather than the standard branch and bound techniques. This new technique used branching on both discrete and continuous variables. The integrality gap, however, remained large.

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

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

2.10 Short-term scheduling methods based on the SSN

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

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

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

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

2.12 More recent scheduling methodologies

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

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

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

2.13 Heat integration in batch plants

Energy usage in multipurpose batch plants can be reduced through the use of heat integration. Heat integration in a batch process is complicated by the fact that it is constrained both by temperature and by time. Direct heat integration as well as storage of heat using a heat transfer fluid for indirect heat integration can be combined to decrease external utility usage. The inclusion of heat storage instead of only direct heat integration leads to more flexibility in the process and therefore improved energy usage.

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

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

2.14 Pinch analysis adapted for batch plants

Early techniques for heat integration in batch processes were based on pinch analysis, which was originally developed for heat integration in continuous plants at steady state. Variations of the technique for batch processes still appear in literature. The major drawback of these techniques is their reliance on a predefined schedule, which leads to suboptimal results.

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

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

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

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

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

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

2.15 Mathematical techniques using a predefined schedule

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

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

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

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

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

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

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

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

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

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

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

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

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

2.16 Simultaneous scheduling and heat integration approaches

For a more optimal solution, scheduling and heat integration may be combined into an overall problem. However, models may be simplified in order to avoid excessive solution times.

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

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

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

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

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

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

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

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

2.17 Specific heat integration applications

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

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

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

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

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

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

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

Majozi (2009) combined both direct and indirect heat integration and applied the model to an agrochemical facility. Savings of more than 75% in external steam consumption in the plant were achieved.

2.18 Heat storage

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

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

The benefit of using direct heat integration over indirect heat integration depends largely on cost. The capital costs of an indirect heat exchanger network include the area of the heat exchangers, a heat storage vessel and the fixed costs of the heat exchangers, for example piping. Using indirect heat integration, two heat exchangers are required and temperature driving forces are split between them. With direct heat integration only one heat exchanger is required and a heat storage vessel is not necessary (Kemp, 1990). Methods for simplifying heat exchanger networks then become important, such as eliminating small, uneconomic heat exchangers.

The cost of including a heat storage system in an existing facility becomes a large part of the total cost. It is more beneficial to evaluate using heat storage systems in new designs (De Boer *et al.*, 2006). The heat storage system should have a high rate of use to be more economical.

2.19 Heat integration formulation based on SSN (Majozi, 2009)

Majozi (2006) presented a formulation for direct heat integration and later extended it to include heat storage for indirect heat integration (Majozi, 2009). This model was ideal for multiproduct plants, but could not adequately address multipurpose facilities. This formulation also included the heat storage size and initial heat storage temperature as fixed parameters. Although this led to a MILP formulation, suboptimal results were obtained. As a basis for the work presented in this dissertation, this model is now discussed.

The model was based on the following problem statement and the superstructure in Figure 2.4.

Given,

(i) Production scheduling data, including equipment capacities, duration of tasks, the time horizon of interest, product recipes, cost of starting materials and selling price of the final products,

(ii) Hot duties for tasks requiring heating and cold duties for tasks that require cooling,

(iii) Cost of cooling water and steam,
(iv) Operating temperatures of the heat sources and heat sinks,
(v) Minimum allowable temperature differences,

Determine the optimal production schedule resulting in minimum energy usage.

The heat transfer fluid remains in its storage vessel while the process fluid is pumped around when heat is to be transferred. Each task is allowed to operate in either integrated or stand alone mode. Each unit may receive direct or indirect heat integration as well as external heating or cooling.

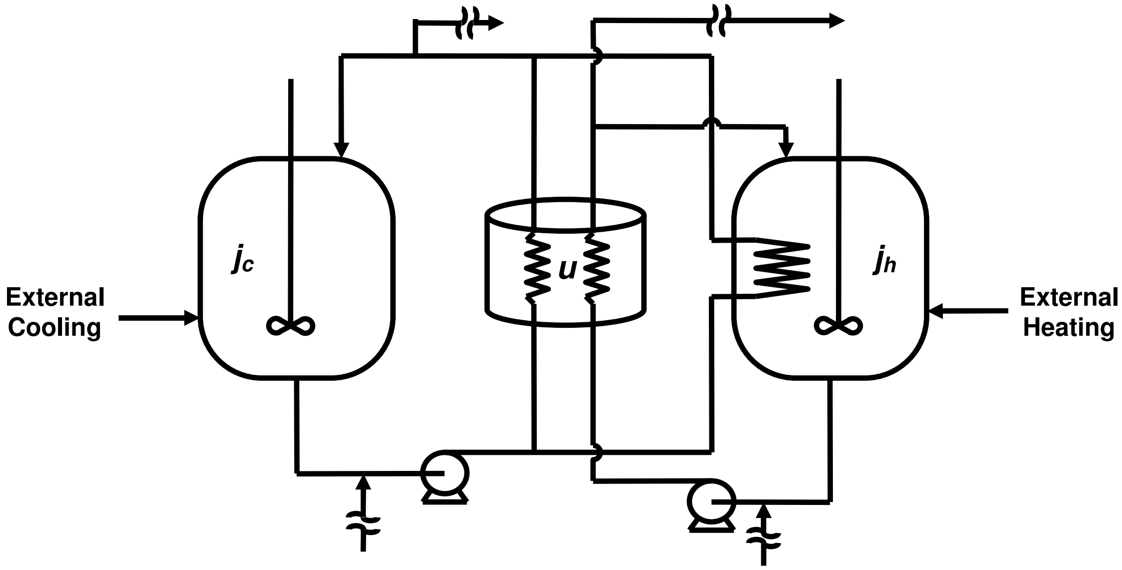

Figure 2.4. Superstructure for the mathematical model.

The mathematical model comprises the following sets, variables and parameters:

Sets

U = $\{u \mid u$ is a heat storage unit$\}$
J = $\{j \mid j$ is a processing unit$\}$

J_c = $\{ j_c \mid j_c$ is a processing unit that requires cooling$\} \subset J$

J_h = $\{ j_h \mid j_h$ is a processing unit that requires heating$\} \subset J$

P = $\{ p \mid p$ is a time point$\}$

$S_{in,j}$ = $\{ s_{in,j} \mid s_{in,j}$ is an input stream to a processing unit$\}$

$S_{out,j}$ = $\{ s_{out,j} \mid s_{out,j}$ is an output stream from a processing unit$\}$

Continuous variables

$t_p\left(s_{out,j}, p\right)$ = time at which a stream is produced from unit j

$t_u\left(s_{in,j}, p\right)$ = time at which a stream enters unit j

$T_0(u, p)$ = initial temperature in heat storage unit u at time point p

$T_f(u, p)$ = final temperature in heat storage unit u at time point p

$CW(j, p)$ = external cooling required by unit j at time point p

$ST(j, p)$ = external heating required by unit j at time point p

$Q(j, u, p)$ = heat exchanged with heat storage unit u at time point p

Binary variables

$$y(j,u,p) = \begin{cases} 1 \leftarrow \text{if unit } j \text{ is integrated with storage unit } u \text{ at time point } p \\ 0 \leftarrow \text{otherwise} \end{cases}$$

$$x(j,j',p) = \begin{cases} 1 \leftarrow \text{if unit } j \text{ is integrated with unit } j' \text{ at time point } p \\ 0 \leftarrow \text{otherwise} \end{cases}$$

$$y\left(s_{in,j}, p\right) = \begin{cases} 1 \leftarrow \text{if unit } j \text{ is active at time point } p \\ 0 \leftarrow \text{otherwise} \end{cases}$$

Parameters

$T(j)$ = operating temperature for processing unit j

$\tau(j)$ = duration of operation j in standalone mode

$\tau'(j, j')$ = duration of operation j when directly heat integrated

$\tau''(j,u)$ = duration of operation j when integrated with storage

$\Delta T^{\min}$ = minimum allowable thermal driving force

$Q(j)$ = amount of heat required by or removed from the operating unit j

$M(u)$ = capacity of heat storage unit u

The variables in the model are time dependent as represented by the index p which represents a time point. Also, as in all batch processes, streams are given by amounts rather than flowrates.

Scheduling constraints can be found in the literature (Majozi & Zhu, 2001). Constraints (2.1) to (2.17) represent the heat integration with heat storage model (Majozi, 2009).

Constraints (2.1) and (2.2) are active simultaneously and ensure that only one pair of units will be involved if direct heat integration takes place. This is a practical consideration in order to simplify process operability as batch processes tend to be labour-intensive. Also, if two units are to be heat integrated at a given time point, they must both be active at that time point.

$$\sum_{j' \in J_c} x(j, j', p) \le y(s_{in,j}, p), \qquad \forall p \in P, j \in J_h, s_{in,j} \in S_{in,j} \tag{2.1}$$

$$\sum_{j \in J_h} x(j, j', p) \le y(s_{in,j'}, p), \qquad \forall p \in P, j \in J_c, s_{in,j'} \in S_{in,j} \tag{2.2}$$

Constraints (2.3) to (2.5) quantify the amount of heat transferred to and received from storage, respectively. If there is no heat integration between a processing unit and storage, the amount of heat in storage remains unchanged. Constraint (2.3) is active at the beginning of the time horizon, $p0$. Constraints (2.4) and (2.5) will be active over the remainder of the time horizon, where p is the current time point and $p-1$ is the previous time point.

$$Q(j,u,p0) = M(u)c_p\left(T_f(u,p1) - T_{Start}\right)y(j,u,p0), \quad \forall j \in J_c \subset J, u \in U \tag{2.3}$$

$$Q(j,u,p-1) = M(u)c_p\left(T_f(u,p) - T_0(u,p-1)\right)y(j,u,p-1),$$
$$\forall j \in J_c \subset J, p \in P, p > p0, u \in U \tag{2.4}$$

$$Q(j',u,p-1) = M(u)c_p\left(T_0(u,p-1) - T_f(u,p)\right)y(j',u,p-1),$$
$$\forall j \in J_h \subset J, p \in P, p > p0, u \in U \tag{2.5}$$

Constraint (2.6) ensures that one unit is heat integrated with one heat storage vessel at any point in time. This is also in consideration of practical operability of the batch process.

$$\sum_{j \in J_c} y(j,u,p) + \sum_{j' \in J_h} y(j',u,p) \le 1, \qquad \forall p \in P, u \in U \tag{2.6}$$

Constraints (2.7) and (2.8) ensure the temperature of heat storage does not change if it is not heat integrated. These constraints are similar to constraints (2.3) to (2.5) except for temperature instead of heat.

$$T_0(u,p-1) \le T_f(u,p) + \max_j\{T(j)\}\left(\sum_{j \in J_c} y(j,u,p-1) + \sum_{j' \in J_h} y(j',u,p-1)\right),$$
$$\forall p \in P, p > p0, u \in U \tag{2.7}$$

$$T_0(u,p-1) \geq T_f(u,p) - \max_j\{T(j)\}\left(\sum_{j\in J_c} y(j,u,p-1) + \sum_{j'\in J_h} y(j',u,p-1)\right),$$
$$\forall p \in P, p > p0, u \in U \qquad (2.8)$$

It can be seen that constraints (2.3) to (2.8) concern the relationship between the heat and the temperature of heat storage.

Constraint (2.9) ensures the initial temperature in heat storage at any time point is the same as the final temperature at the previous time point. This condition will always be true whether or not heat integration took place in the previous time point.

$$T_0(u,p) = T_f(u,p-1), \qquad \forall p \in P, u \in U \qquad (2.9)$$

Constraints (2.10) and (2.11) ensure minimum temperature driving forces are obeyed. Constraint (2.10) applies for heat integration between heat storage and a heat source, while constraint (2.11) applies for heat integration between heat storage and a heat sink.

$$T(j) - T_f(u,p) \geq \Delta T^{\min} - \max_j\{T(j)\}(1 - y(j,u,p-1)),$$
$$\forall p \in P, p > p0, j \in J_c \subset J, u \in U \qquad (2.10)$$

$$T_f(u,p) - T(j) \geq \Delta T^{\min} - \max_j\{T(j)\}(1 - y(j,u,p-1)),$$
$$\forall p \in P, p > p0, j \in J_h \subset J, u \in U \qquad (2.11)$$

Constraint (2.12) states that cooling of any heat source will be either by direct heat integration, external cooling or heat integration with storage. Constraint (2.13) is similar except it is for a heat sink.

$$Q(j)y(s_{in,j},p) = Q(j,u,p) + CW(j,p) + \sum_{j'\in J_h} \min_{j,j'}\{Q(j),Q(j')\}x(j,j',p),$$
$$\forall j \in J_c \subset J, p \in P, u \in U \tag{2.12}$$

$$Q(j)y(s_{in,j},p) = Q(j,u,p) + ST(j,p) + \sum_{j\in J_c} \min_{j,j'}\{Q(j),Q(j')\}x(j,j',p),$$
$$\forall j \in J_h \subset J, p \in P, u \in U \tag{2.13}$$

Constraints (2.14) and (2.15) ensure that if a unit is directly heat integrated with another unit, it cannot be simultaneously integrated with heat storage. This condition also simplifies operability of the process.

$$\sum_{j'\in J_h} x(j,j',p) + y(j,u,p) \le 1, \qquad \forall j \in J_c \subset J, p \in P, u \in U \tag{2.14}$$

$$\sum_{j\in J_c} x(j,j',p) + y(j',u,p) \le 1, \qquad \forall j' \in J_h \subset J, p \in P, u \in U \tag{2.15}$$

Constraint (2.16) is a feasibility constraint ensuring that if a unit is not integrated with storage, the associated duty should not exist.

$$\delta y(j,u,p) \le Q(i,u,p) \le \max_{j\in J}(Q(j),Q(j'))y(j,u,p) \tag{2.16}$$

Constraint (2.17) accounts for the variation in duration due to the heat integration mode. The duration will depend on the temperature driving forces available and will differ depending on whether operation occurs in standalone mode or whether direct or indirect heat integration takes place.

$$t_p(s_{out,j},p) = t_u(s_{in,j},p-1) + \tau(j)\left(1 - y(j,j',p) - y(j,u,p)\right)$$
$$+\tau''(j,u)\,y(j,u,p) + \tau'(j,j')\,y(j,j',p),$$
$$\forall j \in J, p \in P, u \in U, s_{in,j}, s_{out,j} \in S \qquad (2.17)$$

All these constraints are linear except constraints (2.3) to (2.5) which have nonconvex bilinear terms. The bilinear terms are due to the multiplication of a continuous variable with a binary variable. The overall model is therefore a nonconvex MINLP for which a globally optimal solution cannot be guaranteed. This type of bilinearity can be removed, however, using the Glover transformation (Glover, 1975). This is discussed in Appendix A.

The formulation for heat integration using heat storage can be used to determine an optimal schedule which also minimises external utility usage. The model is a MILP if the storage size is fixed.

2.20 Conclusions

The productivity and revenue of a plant can be enhanced by proper scheduling, especially in multipurpose batch plants. Various methods exist and differ mainly with regards to the representation of the flowsheet and the time horizon of interest. The SSN formulation of Majozi and Zhu (2001) has been proven to reduce the number of binary variables, which as a rule of thumb reduces computational time.

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

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

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

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

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

2.21 References

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CHAPTER 3

MATHEMATICAL MODEL

3.1 Introduction

This chapter gives the development of the mathematical model for heat integrating multipurpose batch plants combining direct heat integration and heat storage, over short time horizons. The heat storage capacity and initial temperature are optimisation variables. Time is treated as a variable instead of using a predefined schedule. Batch sizes and processing times are fixed. The linearisation of trilinear terms which arise in the model is discussed. Consideration is also given of heat losses from the idle heat storage vessel.

3.2 Heat integration model

The State Sequence Network (SSN) recipe representation and an uneven discretisation of the time horizon were used to model the process (Majozi & Zhu, 2001). This has proven to result in fewer binary variables compared to models based on other representations.

The model is based on the superstructure in Figure 3.1. The symbols are as defined thereafter. Each task may operate using either direct or indirect heat integration. Tasks may also operate in standalone mode, using only external utilities. This may be required for control reasons or when thermal driving forces or time do not allow for heat integration. If either direct or indirect heat integration is not sufficient to satisfy the required duty, external utilities may make up for any deficit.

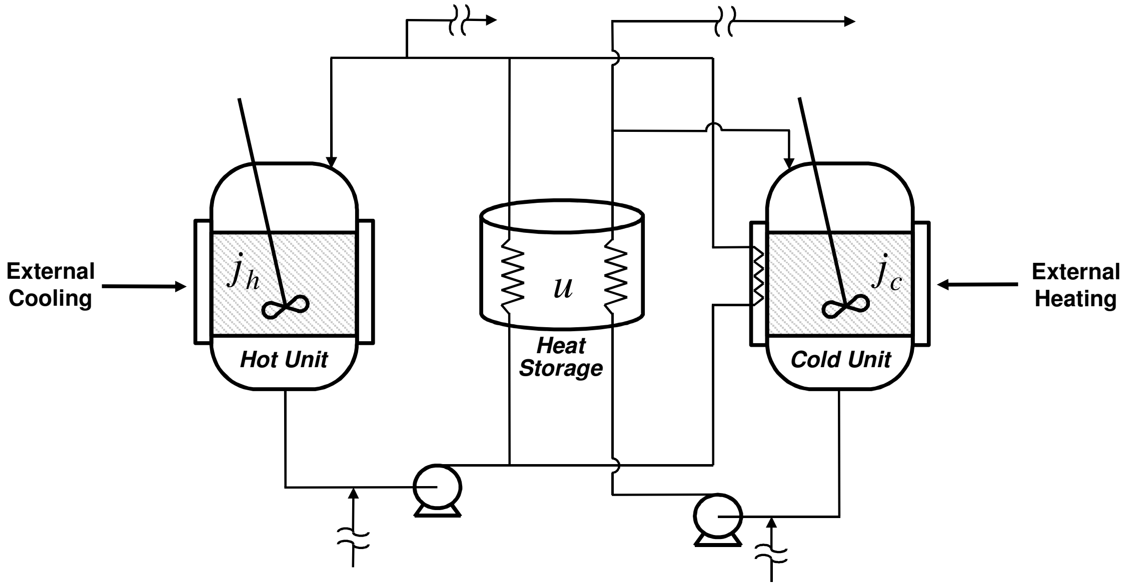

Figure 3.1. Superstructure for mathematical model.

The mathematical model comprises the following sets, variables, parameters and constraints:

Sets

J = $\{ j \mid j$ is a processing unit$\}$

J_c = $\{ j_c \mid j_c$ is a processing unit which may conduct tasks requiring heating$\}$ $\subset J$

J_h = $\{ j_h \mid j_h$ is a processing unit which may conduct tasks requiring cooling$\}$ $\subset J$

P = $\{ p \mid p$ is a time point$\}$

S = $\{ s \mid s$ is any state$\}$

$S_{in,j}$ = $\{ s_{in,j} \mid s_{in,j}$ is an input stream to a processing unit$\}$ $\subset S$

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

Continuous variables

$A_1(u)$ = area for convective heat transfer from heat transfer medium

$A_3(u)$ = area for convective heat transfer to environment

$cw(s_{in,j_h}, p)$ = external cooling required by unit j_h conducting the task corresponding to state s_{in,j_h} at time point p

$L(u)$ = height of heat storage vessel

$Q(s_{in,j}, u, p)$ = heat exchanged with heat storage unit u at time point p

$\dot{Q}_{loss}(u, p)$ = rate of heat loss from idle heat storage unit

$R_{conv_1}(u)$ = convective resistance of heat transfer medium

$R_{conv_3}(u)$ = convective resistance of ambient air

$R_{ins}(u)$ = conductive resistance of insulation

$R_{ves}(u)$ = conductive resistance of heat storage vessel

$R_{tot}(u)$ = thermal resistance for heat storage unit

$st(s_{in,j_c}, p)$ = external heating required by unit j_c conducting the task corresponding to state s_{in,j_c} at time point p

$\Delta\dot{T}(u, p)$ = rate of temperature drop in heat storage unit u due to heat losses

$T_{\infty_{in}}(u, p)$ = steady state temperature equal to the final temperature in the heat storage vessel, $T_f(u, p)$

$T_0(u, p)$ = initial temperature in heat storage unit u at time point p

$T_f(u, p)$ = final temperature in heat storage unit u at time point p

$\Delta t(p)$ = time interval over which heat loss takes place

$t_0(s_{in,j}, u, p)$ = time at which heat storage unit commences activity

$t_f(s_{in,j}, u, p)$ = time at which heat storage unit ends activity

$t_u(s_{in,j}, p)$ = time at which a stream enters unit j

$V(u)$ = volume of heat storage unit u

$W(u)$ = capacity of heat storage unit u

$\Gamma(s_{in,j}, u, p)$ = Glover Transformation variable

$\Psi(s_{in,j}, u, p)$ = Reformulation-Linearisation variable

Binary variables

$$x(s_{in,j_c}, s_{in,j_h}, p) = \begin{cases} 1 \leftarrow \text{if unit } j_c \text{ conducting the task corresponding to state } s_{in,j_c} \\ \qquad \text{is integrated with unit } j_h \text{ conducting the task} \\ \qquad \text{corresponding to state } s_{in,j_h} \text{ at time point } p \\ 0 \leftarrow \text{otherwise} \end{cases}$$

$$y(s_{in,j}, p) = \begin{cases} 1 \leftarrow \text{if state } s \text{ is used in unit } j \text{ at time point } p \\ 0 \leftarrow \text{otherwise} \end{cases}$$

$$z(s_{in,j}, u, p) = \begin{cases} 1 \leftarrow \text{if unit } j \text{ conducting the task corresponding to state } s_{in,j} \text{ is} \\ \qquad \text{integrated with storage unit } u \text{ at time point } p \\ 0 \leftarrow \text{otherwise} \end{cases}$$

Parameters

c_p = specific heat capacity of heat storage fluid

$E(s_{in,j})$ = amount of heat required by or removed from unit j conducting the task corresponding to state $s_{in,j}$

h_1 = convective heat transfer coefficient for free convection of liquids

h_3 = convective heat transfer coefficient for free convection of gases

k_{ins} = thermal conductivity of insulation

k_{ves} = thermal conductivity of heat storage vessel

M = any large number

r_1 = inside radius of heat storage vessel

r_2 = outside radius of heat storage vessel

r_3 = outside radius of insulation

$T(s_{in,j})$ = operating temperature for processing unit j conducting the task corresponding to state $s_{in,j}$

T^L = lower bound for heat storage temperature

T^U = upper bound for heat storage temperature

$\Delta T^{\min}$ = minimum allowable thermal driving force

$T_{\infty_{out}}$ = steady state ambient temperature

$\tau(s_{in,j})$ = duration of the task corresponding to state $s_{in,j}$ conducted in unit j

W^L = lower bound for heat storage capacity

W^U = upper bound for heat storage capacity

Constraints

In addition to the necessary short-term scheduling constraints (Majozi & Zhu, 2001), Constraints (3.1) to (3.22) constitute the heat integration model, useful for multipurpose batch processes with fixed batch sizes and fixed processing times. Both direct and indirect heat integration are considered. The model aims to optimise the production schedule and the heat integration simultaneously. This gives the potential to find better solutions, compared to using a fixed, predefined schedule. The formulation is based on previous models in the literature (Majozi, 2006; Majozi, 2009). These models could not adequately address multipurpose facilities, but were ideal for multiproduct cases.

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

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

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

Constraint (3.3) ensures that only one hot or cold unit is heat integrated with one heat storage unit at any point in time. This is to simplify and improve operational efficiency in the plant.

$$\sum_{s_{in,j_c}} z\left(s_{in,j_c}, u, p\right) + \sum_{s_{in,j_h}} z\left(s_{in,j_h}, u, p\right) \le 1, \qquad \forall\ p \in P,\quad u \in U \qquad (3.3)$$

Constraints (3.4) and (3.5) ensure that a unit cannot simultaneously undergo direct and indirect heat integration. This condition simplifies the operation of the process.

$$\sum_{s_{in,j_h}} x\left(s_{in,j_c}, s_{in,j_h}, p\right) + z\left(s_{in,j_c}, u, p\right) \le 1, \qquad \forall\ p \in P,\quad s_{in,j_c} \in S_{in,j},\quad u \in U \quad (3.4)$$

$$\sum_{s_{in,j_c}} x\left(s_{in,j_c}, s_{in,j_h}, p\right) + z\left(s_{in,j_h}, u, p\right) \le 1, \qquad \forall\ p \in P,\quad s_{in,j_h} \in S_{in,j},\quad u \in U \quad (3.5)$$

Constraints (3.6) and (3.7) quantify the amount of heat received from or transferred to the heat storage unit, respectively. There will be no heat received or transferred if the binary variable signifying use of the heat storage vessel, $z\left(s_{in,j}, u, p\right)$, is zero. These constraints are active over the entire time horizon, where p is the current time point and $p-1$ is the previous time point.

$$Q\left(s_{in,j_c},u,p-1\right)=W(u)c_p\left(T_0(u,p-1)-T_f(u,p)\right)z\left(s_{in,j_c},u,p-1\right),$$
$$\forall\ p\in P, p>p0,\quad s_{in,j_c}\in S_{in,j},\quad u\in U \tag{3.6}$$

$$Q\left(s_{in,j_h},u,p-1\right)=W(u)c_p\left(T_f(u,p)-T_0(u,p-1)\right)z\left(s_{in,j_h},u,p-1\right),$$
$$\forall\ p\in P, p>p0,\quad s_{in,j_h}\in S_{in,j},\quad u\in U \tag{3.7}$$

Constraint (3.8) quantifies the heat transferred to the heat storage vessel at the beginning of the time horizon. The initial temperature of the heat storage fluid is $T_0(u,p0)$.

$$Q\left(s_{in,j_h},u,p0\right)=W(u)c_p\left(T_f(u,p1)-T_0(u,p0)\right)z\left(s_{in,j_h},u,p0\right),$$
$$\forall\ s_{in,j_h}\in S_{in,j},\quad u\in U \tag{3.8}$$

Constraint (3.9) ensures that the final temperature of the heat storage fluid at any time point becomes the initial temperature of the heat storage fluid at the next time point. This condition will hold regardless of whether or not there was heat integration at the previous time point.

$$T_0(u,p)=T_f(u,p-1),\qquad \forall\ p\in P,\quad u\in U \tag{3.9}$$

Constraints (3.10) and (3.11) ensure that temperature of heat storage does not change if there is no heat integration with the heat storage unit, unless there is heat loss from the heat storage unit. M is any large number, thereby resulting in an overall “Big M” formulation. If either $z\left(s_{in,j_c},u,p-1\right)$ or $z\left(s_{in,j_h},u,p-1\right)$ is equal to one, Constraint (3.10) and Constraint (3.11) will be redundant. However, if these two binary variables are both zero, the initial temperature at the previous time point will be equal to the final temperature at the current time point if heat losses are ignored. If heat losses are considered, the temperature will drop over the interval for which the vessel remains idle.

$$T_0(u,p-1) \leq T_f(u,p) + \Delta\dot{T}(u,p-1)\Delta t(p) + M\left(\sum_{s_{in,j_c}} z\left(s_{in,j_c},u,p-1\right) + \sum_{s_{in,j_h}} z\left(s_{in,j_h},u,p-1\right)\right), \quad \forall\ p \in P, p > p0, \quad u \in U \tag{3.10}$$

$$T_0(u,p-1) \geq T_f(u,p) + \Delta\dot{T}(u,p-1)\Delta t(p) - M\left(\sum_{s_{in,j_c}} z\left(s_{in,j_c},u,p-1\right) + \sum_{s_{in,j_h}} z\left(s_{in,j_h},u,p-1\right)\right), \quad \forall\ p \in P, p > p0, \quad u \in U \tag{3.11}$$

Constraint (3.12) ensures that minimum thermal driving forces are obeyed when there is direct heat integration between a hot and a cold unit.

$$T\left(s_{in,j_h}\right) - T\left(s_{in,j_c}\right) \geq \Delta T^{\min} - M\left(1 - x\left(s_{in,j_c}, s_{in,j_h}, p-1\right)\right), \quad \forall\ p \in P, p > p0, \quad s_{in,j_c}, s_{in,j_h} \in S_{in,j} \tag{3.12}$$

Constraints (3.13) and (3.14) ensure that minimum thermal driving forces are obeyed when there is heat integration with the heat storage unit. Constraint (3.13) applies for heat integration between heat storage and a heat sink, while constraint (3.14) applies for heat integration between heat storage and a heat source.

$$T_f(u,p) - T\left(s_{in,j_c}\right) \geq \Delta T^{\min} - M\left(1 - z\left(s_{in,j_c},u,p-1\right)\right), \quad \forall\ p \in P, p > p0, \quad s_{in,j_c} \in S_{in,j}, \quad u \in U \tag{3.13}$$

$$T\left(s_{in,j_h}\right) - T_f\left(u,p\right) \geq \Delta T^{\min} - M\left(1 - z\left(s_{in,j_h}, u, p-1\right)\right),$$

$$\forall\ p \in P, p > p0,\ s_{in,j_h} \in S_{in,j},\quad u \in U \qquad (3.14)$$

Constraint (3.15) states that the cooling of a heat source will be satisfied by either direct or indirect heat integration as well as external utility if required.

$$E\left(s_{in,j_h}\right) y\left(s_{in,j_h}, p\right) = Q\left(s_{in,j_h}, u, p\right) + cw\left(s_{in,j_h}, p\right)$$
$$+ \sum_{s_{in,j_c}} \min_{s_{in,j_c},\, s_{in,j_h}} \left\{E\left(s_{in,j_c}\right), E\left(s_{in,j_h}\right)\right\} x\left(s_{in,j_c}, s_{in,j_h}, p\right),$$

$$\forall\ p \in P,\quad s_{in,j_h} \in S_{in,j},\quad u \in U \qquad (3.15)$$

Constraint (3.16) ensures that the heating of a heat sink will be satisfied by either direct or indirect heat integration as well as external utility if required.

$$E\left(s_{in,j_c}\right) y\left(s_{in,j_c}, p\right) = Q\left(s_{in,j_c}, u, p\right) + st\left(s_{in,j_c}, p\right)$$
$$+ \sum_{s_{in,j_h}} \min_{s_{in,j_c},\, s_{in,j_h}} \left\{E\left(s_{in,j_c}\right), E\left(s_{in,j_h}\right)\right\} x\left(s_{in,j_c}, s_{in,j_h}, p\right),$$

$$\forall\ p \in P,\quad s_{in,j_c} \in S_{in,j},\quad u \in U \qquad (3.16)$$

Constraints (3.17) and (3.18) ensure that the times at which units are active are synchronised when direct heat integration takes place. Starting times for the tasks in the integrated units are the same. This constraint may be relaxed for operations requiring preheating or precooling and is dependent on the process.

$$t_u\left(s_{in,j_h}, p\right) \geq t_u\left(s_{in,j_c}, p\right) - M\left(1 - x\left(s_{in,j_c}, s_{in,j_h}, p\right)\right)$$

$$\forall\ p \in P,\quad s_{in,j_c}, s_{in,j_h} \in S_{in,j} \qquad (3.17)$$

$$t_u\left(s_{in,j_h},p\right)\leq t_u\left(s_{in,j_c},p\right)+M\left(1-x\left(s_{in,j_c},s_{in,j_h},p\right)\right)$$
$$\forall\ p\in P,\quad s_{in,j_c},s_{in,j_h}\in S_{in,j} \tag{3.18}$$

Constraints (3.19) and (3.20) ensure that if indirect heat integration takes place, the time a unit is active will be equal to the time a heat storage unit starts either to transfer or receive heat.

$$t_u\left(s_{in,j},p\right)\geq t_0\left(s_{in,j},u,p\right)-M\left(y\left(s_{in,j},p\right)-z\left(s_{in,j},u,p\right)\right)$$
$$\forall\ p\in P,\quad u\in U,\quad s_{in,j}\in S_{in,j} \tag{3.19}$$

$$t_u\left(s_{in,j},p\right)\leq t_0\left(s_{in,j},u,p\right)+M\left(y\left(s_{in,j},p\right)-z\left(s_{in,j},u,p\right)\right)$$
$$\forall\ p\in P,\quad u\in U,\quad s_{in,j}\in S_{in,j} \tag{3.20}$$

Constraints (3.21) and (3.22) state that the time when heat transfer to or from a heat storage unit is finished will coincide with the time the task transferring or receiving heat has finished processing.

$$t_u\left(s_{in,j},p-1\right)+\tau\left(s_{in,j}\right)y\left(s_{in,j},p-1\right)\geq t_f\left(s_{in,j},u,p\right)$$
$$-M\left(y\left(s_{in,j},p-1\right)-z\left(s_{in,j},u,p-1\right)\right)$$
$$\forall\ p\in P,p>p0,\quad u\in U,\quad s_{in,j}\in S_{in,j} \tag{3.21}$$

$$t_u\left(s_{in,j},p-1\right)+\tau\left(s_{in,j}\right)y\left(s_{in,j},p-1\right)\leq t_f\left(s_{in,j},u,p\right)$$
$$+M\left(y\left(s_{in,j},p-1\right)-z\left(s_{in,j},u,p-1\right)\right)$$
$$\forall\ p\in P,p>p0,\quad u\in U,\quad s_{in,j}\in S_{in,j} \tag{3.22}$$

3.3 Linearisation

Constraints (3.6), (3.7) and (3.8) have trilinear terms resulting in a nonconvex MINLP formulation. The bilinearity resulting from the multiplication of a continuous variable with a binary variable may be handled effectively with the Glover transformation (Glover, 1975). This is an exact linearisation technique and as such will not compromise the accuracy of the model. The procedure is demonstrated for Constraint (3.7) in Appendix A, and leads to Constraint (3.23).

$$Q\left(s_{in,j_h},u,p-1\right)=W(u)c_p\left(\Gamma_1\left(s_{in,j_h},u,p\right)-\Gamma_2\left(s_{in,j_h},u,p-1\right)\right),$$
$$\forall\ p\in P, p>p0,\quad s_{in,j_h}\in S_{in,j},\quad u\in U \tag{3.23}$$

The heat storage capacity, $W(u)$, is also a continuous variable and is multiplied with the continuous Glover transformation variable. This results in another type of bilinearity, which results in a nonconvex model. A method to handle this is a Reformulation-Linearisation technique (Sherali & Alameddine, 1992) as discussed by Quesada and Grossmann (1995). This is demonstrated for Constraint (3.23), resulting in Constraints (3.24) to (3.30).

Let

$$W(u)\Gamma_1\left(s_{in,j_h},u,p\right)=\Psi_1\left(s_{in,j_h},u,p\right) \tag{3.24}$$

With lower and upper heat storage capacity and temperature bounds known

$$W^L\le W(u)\le W^U \tag{3.25}$$

$$T^L\le\Gamma_1\left(s_{in,j_h},u,p\right)\le T^U \tag{3.26}$$

Then

$$\Psi_1\left(s_{in,j_h},u,p\right)\geq W^L\Gamma_1\left(s_{in,j_h},u,p\right)+T^LW(u)-W^LT^L \tag{3.27}$$

$$\Psi_1\left(s_{in,j_h},u,p\right)\geq W^U\Gamma_1\left(s_{in,j_h},u,p\right)+T^UW(u)-W^UT^U \tag{3.28}$$

$$\Psi_1\left(s_{in,j_h},u,p\right)\leq W^U\Gamma_1\left(s_{in,j_h},u,p\right)+T^LW(u)-W^UT^L \tag{3.29}$$

$$\Psi_1\left(s_{in,j_h},u,p\right)\leq W^L\Gamma_1\left(s_{in,j_h},u,p\right)+T^UW(u)-W^LT^U \tag{3.30}$$

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

The final completely linearised form of Constraint (3.7) can be seen in Constraint (3.31).

$$Q\left(s_{in,j_h},u,p-1\right)=c_p\left(\Psi_1\left(s_{in,j_h},u,p\right)-\Psi_2\left(s_{in,j_h},u,p-1\right)\right)$$
$$\forall\ p\in P, p>p0,\quad s_{in,j_h}\in S_{in,j},\quad u\in U \tag{3.31}$$

The full linearisation procedure is carried out for each of the trilinear terms resulting from Constraints (3.6), (3.7) and (3.8). Bounds on the heat storage capacity will be determined by the available space in the plant, as batch plants usually operate in limited space.

The linearised model is solved as a MILP, the solution of which is then used as a starting point for the exact MINLP model. If the solutions from the two models are equal, the solution is globally optimal, as global optimality can be proven for MILP problems. If the solutions differ, the MINLP solution is locally optimal. The possibility also exists that no feasible starting point is found. The solution algorithm is shown graphically in Figure 3.2.

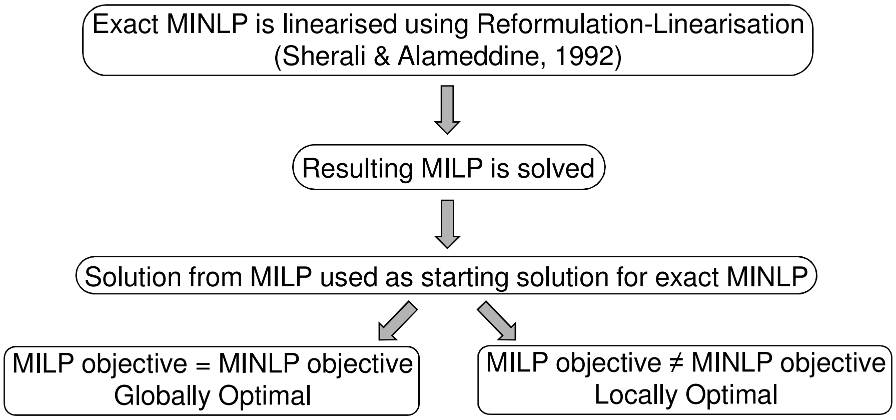

Figure 3.2. Solution algorithm for Reformulation-Linearisation technique.

3.4 Heat loss considerations

Constraint (3.32), which is used in Constraint (3.10) and Constraint (3.11), accounts for heat loss from an idle heat storage vessel. As the temperature drop of heat storage due to heat loss will be minimal, it is assumed the temperature of the fluid has reached steady state and the rate of heat transfer in the time interval is constant. The heat storage vessel may be represented as in Figure 3.3.

$$\Delta\dot{T}(u,p)=\frac{\dot{Q}_{loss}(u,p)}{W(u)c_p} \qquad \forall\ p\in P, p>p0, \quad u\in U \tag{3.32}$$

The idle time for the heat storage vessel, when heat is neither stored nor released, is defined by Constraint (3.33).

$$\Delta t(p)=t_0\left(s_{in,j},u,p\right)-t_f\left(s_{in,j},u,p-1\right)$$
$$\forall\ p\in P, p>p0, \quad s_{in,j_h}\in S_{in,j}, \quad u\in U \tag{3.33}$$

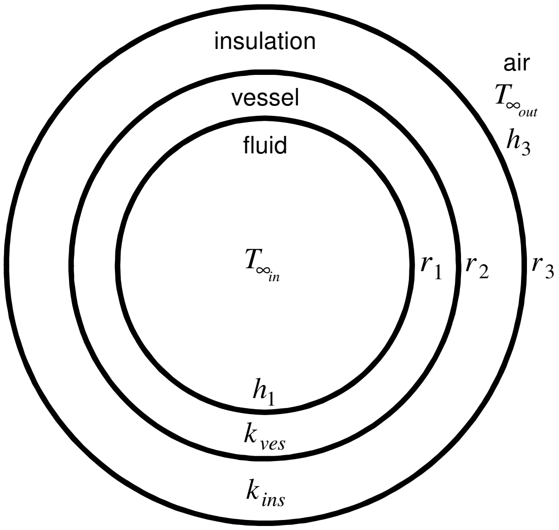

Figure 3.3. Insulated heat storage vessel.

The amount of heat lost to the environment is quantified in Constraint (3.34).

$$\dot{Q}_{loss}(u,p)=\frac{T_{\infty_{in}}(u,p)-T_{\infty_{out}}}{R_{tot}(u)} \qquad \forall\ p\in P, p>p0, \quad u\in U \tag{3.34}$$

$T_{\infty_{in}}$ is equal to the final temperature in the heat storage vessel, $T_f(u,p)$ and $T_{\infty_{out}}$ is the steady state ambient temperature. The total thermal resistance due to convection and conduction is given by Constraint (3.35) with each term defined in Constraint (3.36).

$$R_{tot}(u)=R_{conv_1}(u)+R_{ves}(u)+R_{ins}(u)+R_{conv_3}(u) \qquad \forall\ u\in U \tag{3.35}$$

$$R_{tot}(u)=\frac{1}{h_1A_1(u)}+\frac{\ln\left(\frac{r_2}{r_1}\right)}{2\pi L(u)k_{ves}}+\frac{\ln\left(\frac{r_3}{r_2}\right)}{2\pi L(u)k_{ins}}+\frac{1}{h_3A_3(u)} \qquad \forall\ u\in U \tag{3.36}$$

The internal area for heat loss by convection from the heat transfer medium is given by Constraint (3.37) and the area for convective heat transfer losses to the environment is given in Constraint (3.38).

$$A_1(u) = 2\pi r_1 L(u) \qquad \forall \ u \in U \qquad (3.37)$$

$$A_3(u) = 2\pi r_3 L(u) \qquad \forall \ u \in U \qquad (3.38)$$

If the density of the heat transfer fluid is assumed to be 1000 kg/m^3, the volume in m^3 will be numerically equal to the mass of the storage requirement in tons. This volume is given by Constraint (3.39).

$$W(u) = V(u) = \pi r_1^2 L(u) \qquad \forall \ u \in U \qquad (3.39)$$

The radius of the tank is assumed to be fixed, with the height of the tank allowed to vary.

3.5 References

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CHAPTER 4

RESULTS AND DISCUSSION

4.1 Introduction

The results obtained from applying the heat integration model to two examples are presented. The first example is a problem taken from literature, modified to include heating and cooling tasks in order to explore heat integration opportunities. The second example is an industrial case study. Linearisation and consequences for global optimality are discussed. Effects of heat losses from the idle heat storage vessel are also shown.

4.2 Literature example (Sundaramoorthy & Karimi, 2005)

A scheduling problem was taken from literature and modified to include heating and cooling tasks for the reactions taking place in the process. In this way, opportunities for heat integration were explored. The state task network for the process is shown in Figure 4.1 and the state sequence network is shown in Figure 4.2. The example is for a multipurpose facility and the process requires sharing of equipment and multiple tasks and states.

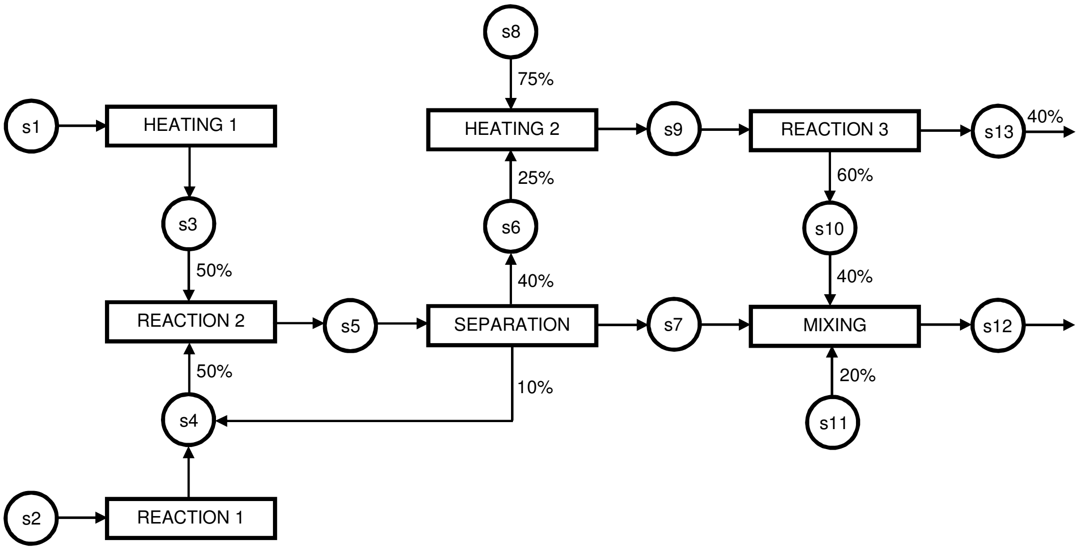

Figure 4.1. State task network of multipurpose batch facility.

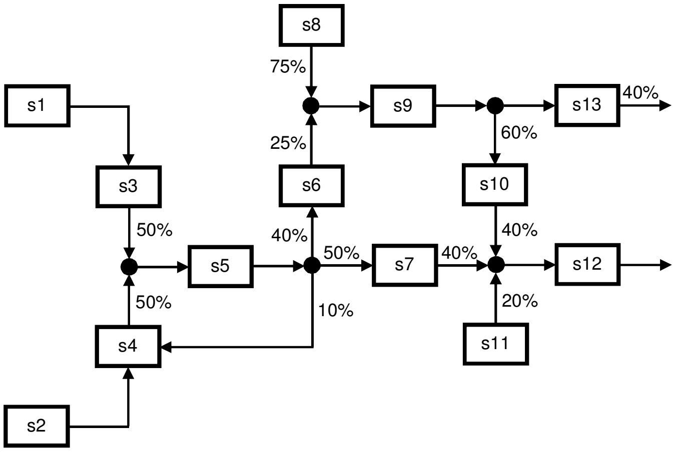

Figure 4.2. State sequence network of multipurpose batch facility.

Scheduling data are shown in Table 4.1 and Table 4.2 (Sundaramoorthy & Karimi, 2005), while heat integration data are shown in Table 4.3. A heat storage fluid with a high heat capacity will provide good temperature control and facilitate easy heat recovery. Heating and cooling requirements for tasks are shown in Table 4.4.

Table 4.1. Scheduling data for literature example.

Unit	Capacity	Suitability	Mean processing time (h)
Heater	100	H1, H2	1, 1.5
Reactor 1	100	RX1, RX2, RX3	2, 1, 2
Reactor 2	150	RX1, RX2, RX3	2, 1, 2
Separator	300	Separation	3
Mixer 1	200	Mixing	2
Mixer 2	200	Mixing	2

Table 4.2. Scheduling data for literature example.

State	Description	Storage capacity (ton)	Initial amount (ton)	Revenue (cu/ton)
s1	Feed 1	unlimited	unlimited	0
s2	Feed 2	unlimited	unlimited	0
s3	Intermediate 1	100	0	0
s4	Intermediate 2	100	0	0
s5	Intermediate 3	300	0	0
s6	Intermediate 4	150	50	0
s7	Intermediate 5	150	50	0
s8	Feed 3	unlimited	unlimited	0
s9	Intermediate 6	150	0	0
s10	Intermediate 7	150	0	0
s11	Feed 4	unlimited	unlimited	0
s12	Product 1	unlimited	0	5
s13	Product 2	unlimited	0	5

Table 4.3. Heat integration data for literature example.

Parameter	Value
Specific heat capacity, c_p (kJ/kg°C)	4.2
Product selling price (cu/ton)	1000
Steam cost (cu/kWh)	10
Cooling water cost (cu/kWh)	2
$\Delta T^{\min}$ (°C)	10
T^L (°C)	20
T^U (°C)	180
W^L (ton)	1
W^U (ton)	3

Table 4.4. Heating/cooling requirements for literature example.

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

Parameters for heat loss considerations may be found in Table 4.5.

Table 4.5. Data for literature example with heat losses.

Parameter	Value
Tank wall thickness (mm)	5
Insulation thickness (mm)	30
r_1 (m)	0.5
r_2 (m)	0.505
r_3 (m)	0.535
h_1 (kW/m^2°C)	0.1
h_3 (kW/m^2°C)	0.02
k_{ves} (kW/m°C)	0.015
k_{ins} (kW/m°C)	0.00005
$T_{\infty_{out}}$ (°C)	20

The batch sizes for all units were fixed at 80% of design capacity. The resulting optimal schedule for the literature example is shown in Figure 4.3. Heat integration is indicated with arrows and one heat storage unit was used.

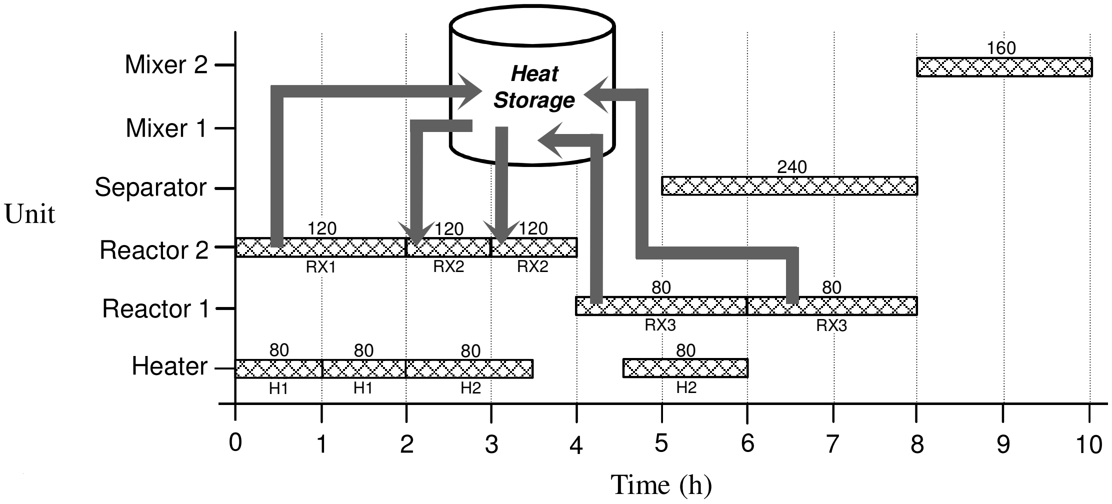

Figure 4.3. Optimal schedule for literature example with heat losses.

The variation in temperature of the heat storage vessel may be seen in Figure 4.4.

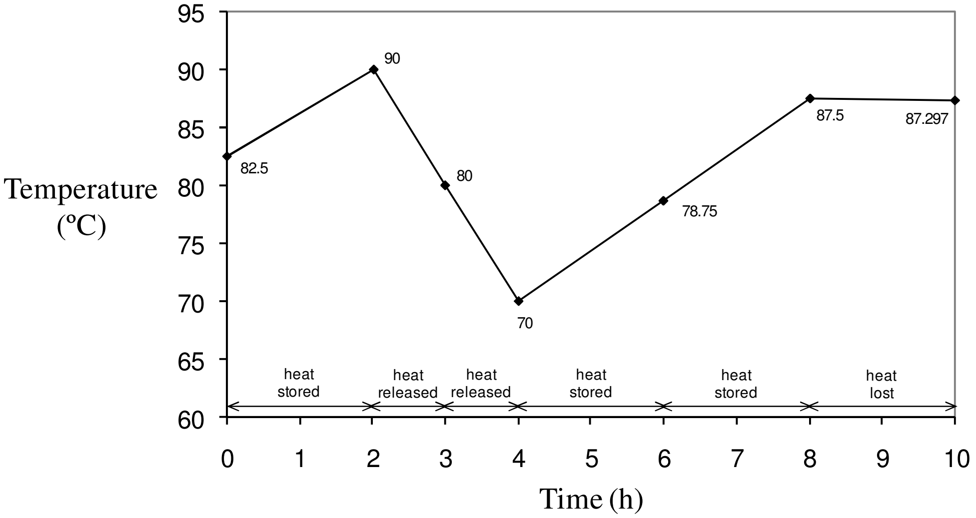

Figure 4.4. Variation in heat storage temperature for literature example.

The results for literature example are summarised in Table 4.6. Heat from the first exothermic reaction was stored and used for heating the second reaction. As seen from the results, there were no opportunities for direct heat integration and using indirect heat integration eliminated the requirement for external utilities. The solution procedure as described previously in Figure 3.2 was used in solving the MINLP problem for the case including heat storage. The result obtained from the linearised model was the same as for the exact model, therefore, the result obtained was globally optimal. CPLEX 9.1.2 was used to solve the linearised model. DICOPT2 was used in the solution of the MINLP problem with CPLEX 9.1.2 as the MIP solver and CONOPT2 as the NLP solver in GAMS 22.0. The problem was solved on a Pentium 4, 3.2 GHz processor with 512 MB RAM. Both the size of the heat storage vessel as well as the initial temperature did not change when heat losses were considered compared to the case where heat losses were disregarded, as the heat storage vessel was only idle at the end of the time horizon.

Table 4.6. Results for literature example.

	No heat integration	**Direct heat integration only**	**Direct and indirect heat integration – optimal heat storage capacity and initial temperature**
Performance index (cost units) [q]	222 000	222 840	224 000
External cold duty (kWh)	200	130	0
External hot duty (kWh)	160	90	0
Heat storage capacity (ton)			1.905
Initial heat storage temperature (ºC)			82.5
CPU time (s)			68
Binary variables			156
Time points			7

[q] Performance Index = Revenue – Utility Costs

4.3 Industrial case study (Majozi & Zhu, 2001)

The flowsheet for the process is shown in Figure 4.5.

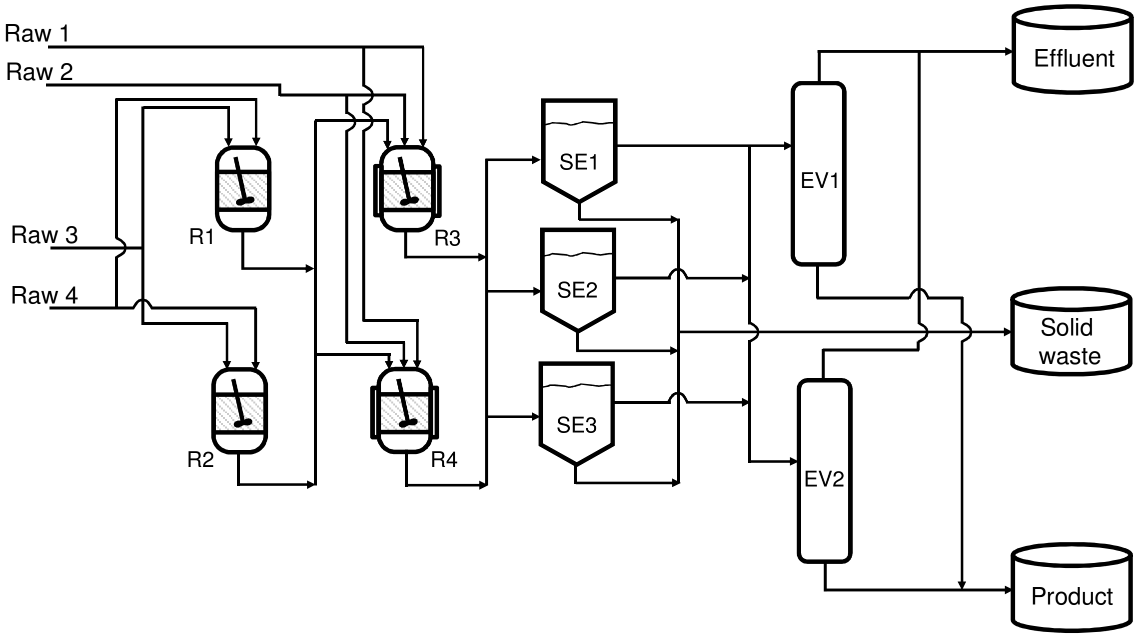

Figure 4.5. Flowsheet for the industrial case study.

The STN for the process is shown in Figure 4.6 and the SSN is shown in Figure 4.7. The scheduling data may be obtained from Tables 4.7, 4.8 and 4.9 (Majozi & Zhu, 2001). The plant consumes 55% of the steam utility in an agrochemical facility. Each of the units processes a fixed batch size of eight tons, 80% of design capacity. The process requires three consecutive chemical reactions which take place in four available reactors. Reaction 1 takes place in either Reactor 1 or Reactor 2 and takes two hours. The intermediate from Reaction 1 is then transferred either to Reactor 3 or Reactor 4, where two consecutive reactions take place. Reaction 2 takes three hours and Reaction 3, one hour. Reaction 2 is highly exothermic and requires almost nine tons of cooling water (equivalent to 100 kWh). For operational purposes, these two consecutive reactions take place in a single reactor. Some of the intermediate from the first of these two reactions can be stored in an intermediate buffer tank prior to the final reaction to improve throughput. Both the second and third reactions form sodium chloride as a byproduct. The intermediate from Reaction 3 is transferred to one of three Settlers, to separate the sodium chloride from the aqueous solution containing the active ingredient. This process takes one hour. This salt-free solution is then transferred to one of two Evaporators, where steam (equivalent to 110 kWh) is used to remove excess water from the product, which takes three hours. This water is dispensed with as effluent. The final product is collected in storage tanks before final formulation, packaging and transportation to customers. This is an example of a sequential, mainly multiproduct process.

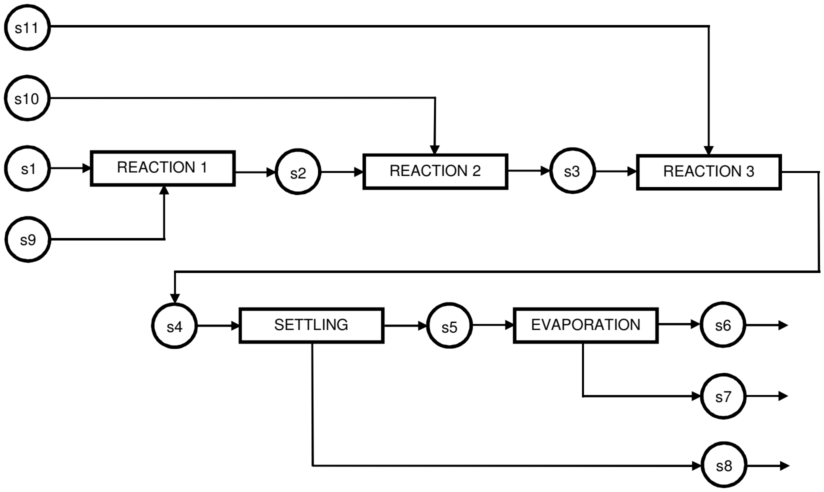

Figure 4.6. State task network of industrial case study.

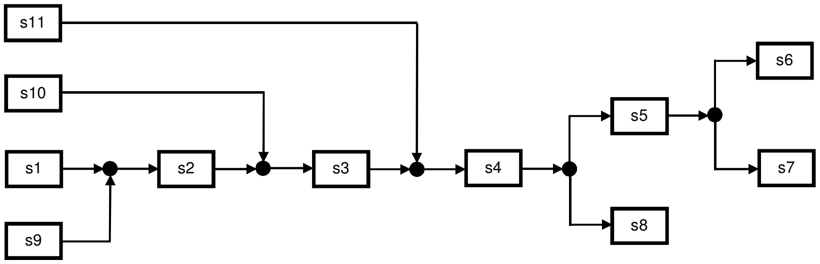

Figure 4.7. State sequence network of industrial case study.

Table 4.7. Scheduling data for industrial case study.

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

Table 4.8. Scheduling data for industrial case study.

State	Storage capacity (ton)	Initial amount (ton)	Revenue (cu/ton)
s1	unlimited	unlimited	0
s2	unlimited	unlimited	0
s3	100	0	0
s4	100	0	0
s5	300	0	0
s6	150	50	0
s7	150	50	0
s8	unlimited	unlimited	0
s9	150	0	0
s10	150	0	0
s11	unlimited	unlimited	0

Table 4.9. Stoichiometric data for industrial case study.

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

The temperatures for the exothermic second reaction (150°C) and endothermic evaporation stage (90°C) allow for possible heat integration.

Necessary heat integration data for the industrial case study may be found in Table 4.10, with heating and cooling requirements summarised in Table 4.11.

Table 4.10. Heat integration data for industrial case study.

Parameter	Value
Specific heat capacity, c_p (kJ/kg°C)	4.2
Product selling price (cu/ton)	10 000
Steam cost (cu/kWh)	20
Cooling water cost (cu/kWh)	8
$\Delta T^{\min}$ (°C)	5
T^L (°C)	20
T^U (°C)	180
W^L (ton)	0.2
W^U (ton)	1

Table 4.11. Heating/cooling requirements for industrial case study.

Reaction	**Type**	**Heating/Cooling Requirement (kWh)**	**Operating Temperature (ºC)**
RX2	exothermic	100 (cooling)	150
Evaporation	endothermic	110 (heating)	90

Heat integration in Figure 4.8 is indicated with arrows. One heat storage unit was used and initially heat losses were not included. Heat is transferred throughout the duration of a task. The heat storage capacity and initial heat storage temperature were optimised. It can be seen from the results that it is possible to reuse energy which was stored previously in the process.

For non-optimal values for the heat storage capacity and initial heat storage temperature, heat was stored, but not reused over the time horizon (Majozi, 2009). The results for different scenarios are summarised in Table 4.12.

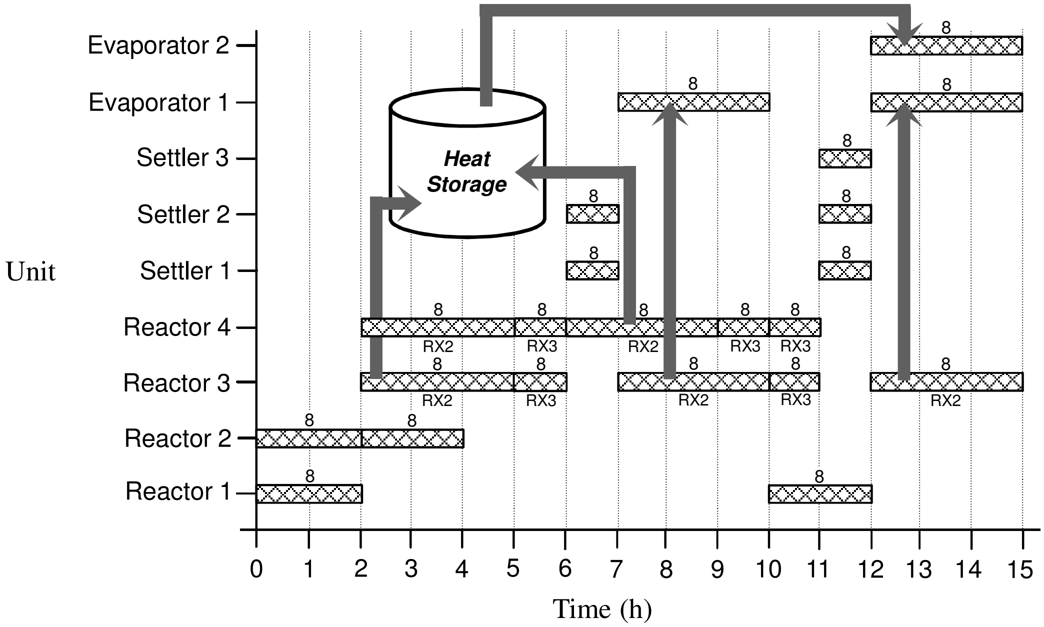

Figure 4.8. Schedule shows improvement in energy usage (no heat losses).

The variation in temperature of the heat storage vessel, disregarding heat losses is shown in Figure 4.9.

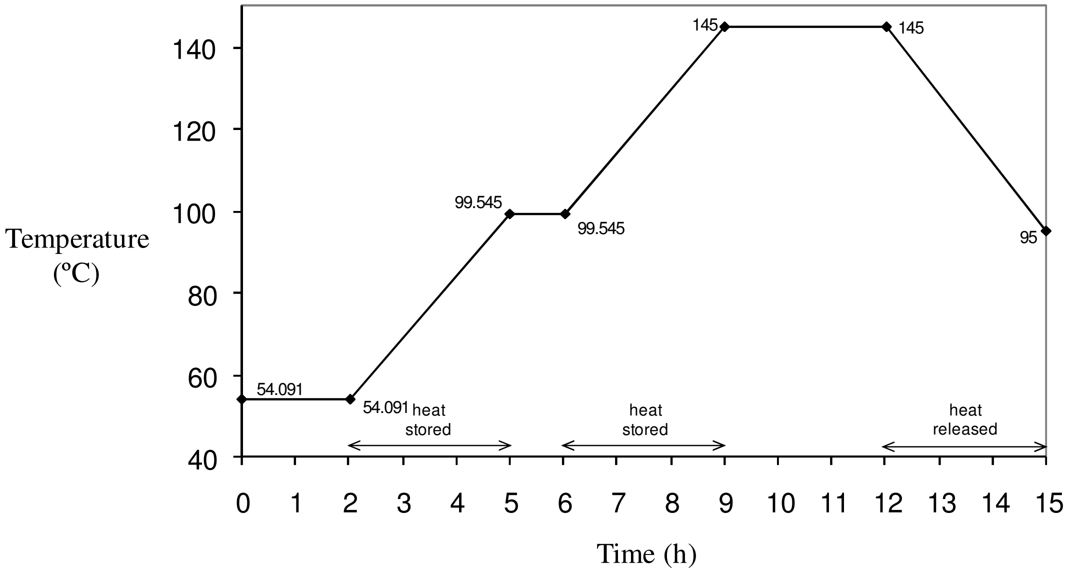

Figure 4.9. Temperature variation in heat storage vessel (no heat losses).

Table 4.12. Results for industrial case study (no heat losses).

	No heat integration	**Direct heat integration only**	**Direct and indirect heat integration (Majozi, 2009)**	**Direct and indirect heat integration – optimal heat storage capacity**
Performance index (cost units) [q]	131 376.471	138 176.471	139776.471	139 976.471
External cold duty (kWh)	400	300	100	100
External hot duty (kWh)	330	30	30	20
Heat storage capacity (ton)			2	0.524
Initial heat storage temperature (°C)			80	54.091
CPU time (s)			2805.2	95396
Binary variables				194
Time points				11

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[q] Performance index = Revenue – utility costs

The solution procedure as described previously in Figure 3.2 was used in solving the MINLP problem for the case including heat storage. The result obtained from the linearised model was the same as for the exact model meaning the result obtained was globally optimal. CPLEX 9.1.2 was used to solve the linearised model, while DICOPT2 was used in the solution of the MINLP problem with CPLEX 9.1.2 as the MIP solver and CONOPT as the NLP solver in GAMS 22.0. The problem was solved on a Pentium 4, 3.2 GHz processor with 512 MB RAM.

Heat loss considerations

Heat losses from the idle heat storage tank for the industrial case study were included with the parameters in Table 4.13. The time horizon of interest was decreased to 10 hours in order to reduce the solution time.

Table 4.13. Data for industrial case study with heat losses accounted for.

Parameter	Value
Tank wall thickness (mm)	5
Insulation thickness (mm)	30
r_1 (m)	0.5
r_2 (m)	0.505
r_3 (m)	0.535
h_1 (kW/m^2°C)	0.1
h_3 (kW/m^2°C)	0.02
k_{ves} (kW/m°C)	0.015
k_{ins} (kW/m°C)	0.00005
$T_{\infty_{out}}$ (°C)	20

The results may be obtained from Table 4.14.

Table 4.14. Results for industrial case study with heat losses.

	No heat loss	**Heat loss**
Performance index (cost units)	46258.824	46258.824
External cold duty (kWh)	100	100
External hot duty (kWh)	0	0
Heat storage capacity (ton)	0.524	0.530
Height of heat storage vessel (m)	0.667	0.675
Initial heat storage temperature (ºC)	99.545	100.298

The Gantt chart for the case where heat losses from the heat storage vessel were considered can be seen in Figure 4.10.

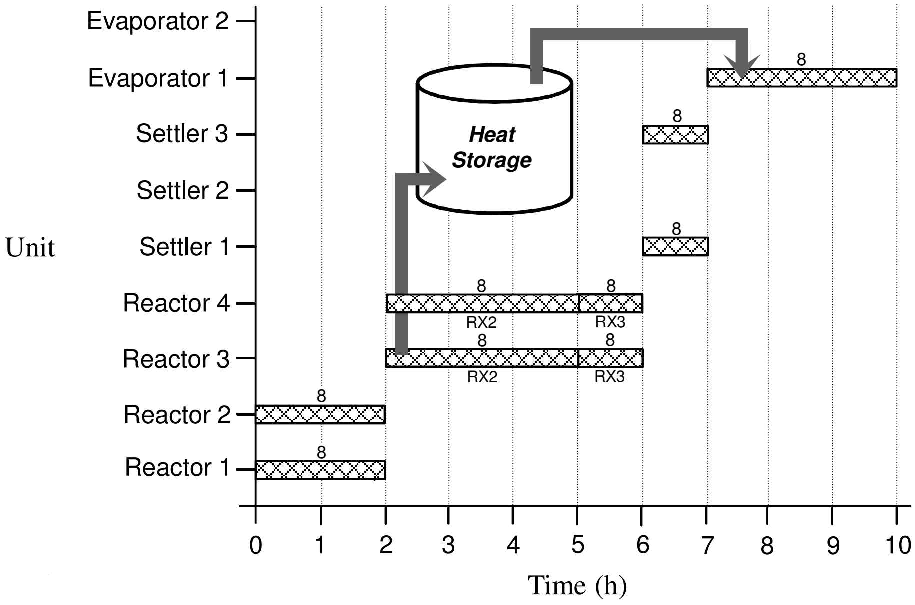

Figure 4.10. Optimal schedule over shorter time horizon.

As can be seen from the results in Table 4.14, the shorter time horizon requires a higher starting temperature when compared to the horizon of 15 hours. This is due to the heat storage vessel being unable to receive heat from the exothermic reaction twice. However, heat is still able to be transferred to the endothermic evaporation stage. The variation in the temperature of the heat storage vessel with heat losses can be seen in Figure 4.11.

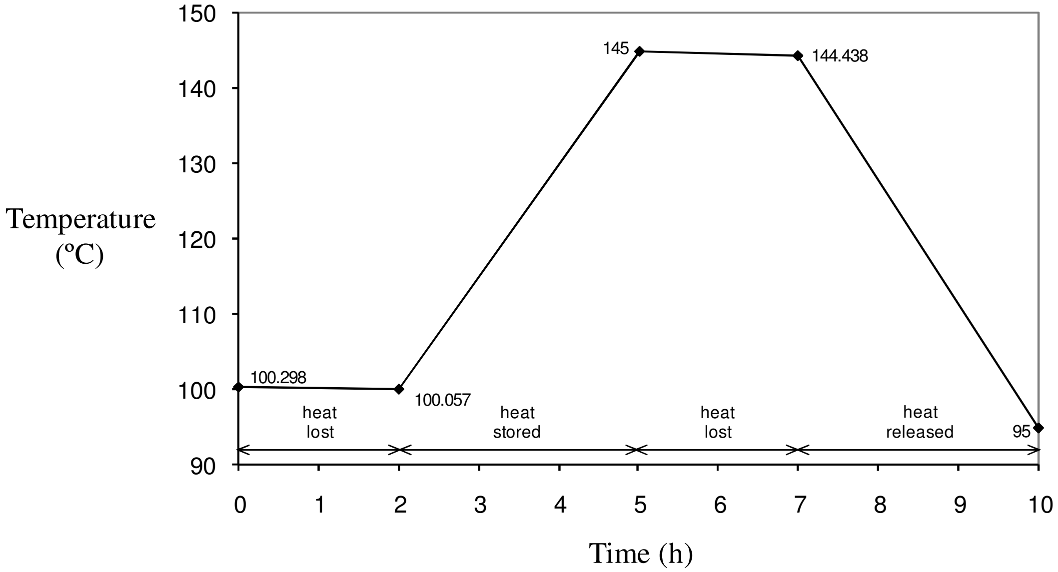

Figure 4.11. Temperature variation in heat storage vessel with heat losses.

The heat losses from the heat storage vessel depend on both the initial temperature in the vessel as well as the time over which the vessel is idle. As can be seen from Figure 4.11, the temperature gradient is steeper from 5 to 7 hours {(145 - 144.438)/2 = 0.281} when compared to 0 to 2 hours, {(100.298 – 100.057)/2 = 0.121} due to the higher initial temperature in the heat storage vessel. The capacity of the heat storage tank as well as the initial temperature were increased when heat losses were considered. The objective function and external hot and cold utility requirements were, however, unaffected.

The temperature drop due to heat losses may be considered negligible for a well insulated heat storage vessel over short time horizons if temperatures are low.

4.4 References

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CHAPTER 5

CONCLUSIONS

A heat integration formulation for multipurpose batch plants was presented. The methodology ensures that the operating schedule and heat integration are optimised simultaneously. Both direct and indirect heat integration were considered. Emphasis was placed on the optimal design of the heat storage vessel in terms of heat storage capacity and initial heat storage temperature. Consideration of heat losses from the idle heat storage vessel was also included.

Results from a modified literature example showed that no external utilities were required when direct heat integration was combined with indirect heat integration, with optimal heat storage capacity and initial heat storage temperature. The requirement for external hot utility in an industrial case study was decreased by 33% when using optimal values compared to using known parameters for the heat storage capacity and initial heat storage temperature. Solutions obtained for both examples were globally optimal.

For the industrial case study, the initial temperature and heat storage capacity increased when considering heat losses, but the objective value remained the same. The temperature drop in the heat storage vessel due to heat losses was dependent on the temperature in the heat storage vessel (a gradient of 0.281 for an initial temperature of 145°C compared to a gradient of 0.121 for an initial temperature of 100.298°C). Heat losses may be considered negligible for a well insulated vessel over short time horizons if temperatures are low.

Appendix A: Glover transformation (Glover, 1975)

From Constraint (3.7),

Let

$$T_f(u,p)z(s_{in,j_h},u,p-1)=\Gamma_1(s_{in,j_h},u,p) \tag{A1}$$

With lower and upper temperature bounds known

$$T^L \le T_f(u,p) \le T^U \tag{A2}$$

Then

$$\Gamma_1(s_{in,j_h},u,p) \ge T_f(s_{in,j_h},u,p)-T^U\left(1-z(s_{in,j_h},u,p-1)\right) \tag{A3}$$

$$\Gamma_1(s_{in,j_h},u,p) \le T_f(s_{in,j_h},u,p)+T^L\left(1-z(s_{in,j_h},u,p-1)\right) \tag{A4}$$

$$\Gamma_1(s_{in,j_h},u,p) \ge z(s_{in,j_h},u,p-1)T^L \tag{A5}$$

$$\Gamma_1(s_{in,j_h},u,p) \le z(s_{in,j_h},u,p-1)T^U \tag{A6}$$

The result from the Glover transformation for Constraint (3.7) is seen in Constraint (A7) and includes the addition of one new type of continuous variable and four new types of continuous constraints.

$$Q(s_{in,j_h},u,p-1)=W(u)c_p\left(\Gamma_1(s_{in,j_h},u,p)-\Gamma_2(s_{in,j_h},u,p-1)\right),$$
$$\forall\ p\in P, p>p0, \quad s_{in,j_h}\in S_{in,j}, \quad u\in U \tag{A7}$$