Augmented Heat Integration in Multipurpose Batch Plants Using Multiple Heat Storage Vessels

Thokozani Majozi

Abstract Energy minimisation in batch plants has garnered popularity over the past few decades, leading to direct and indirect heat integration techniques being formulated for multipurpose batch plants through the utilisation of mathematical formulations and insight-based methods. Some mathematical formulations utilise predetermined scheduling frameworks which may result in suboptimal results, whilst other formulations only use one heat storage vessel which may cause limitations in the plant. The work presented in this chapter is aimed at minimising energy consumption in multipurpose batch plants by exploring both direct and indirect heat integration through multiple heat storage vessels. It investigates the optimal number of heat storage vessels as well as design parameters, i.e. size and initial temperature of vessels. The cost of the heat storage vessels is considered within the model. The model is applied to two case studies resulting in significant increase in profits.

Keywords Batch plants · Heat integration · Energy · Minimisation
Heat storage · Optimisation

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

Sets

J	$\{j \mid j$ processing unit$\}$
J_c	$\{j_c \mid j_c$ cold processing unit$\}$
J_h	$\{j_h \mid j_h$ hot processing unit$\}$
P	$\{p \mid p$ time point$\}$
S_{jh}^{in}	$\{s_{jh}^{in} \mid s_{jh}^{in}$ task which needs cooling$\}$
S_{jc}^{in}	$\{s_{jc}^{in} \mid s_{jc}^{in}$ task which needs heating$\}$
S_{j}^{in}	$\{s_{j}^{in} \mid s_{j}^{in}$ any task$\}$

T. Majozi (✉)
School of Chemical and Metallurgical Engineering, University of Witwatersrand,
1 Jan Smuts Avenue, Braamfontein, Johannesburg 2001, South Africa
e-mail: thokozani.majozi@wits.ac.za

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S_p $\{s_p | s_p$ any product$\}$
V $\{v | v$ is a heat storage vessel$\}$

Variables

$Ec(s_{jc}^{in}, p)$	Duty of task which needs heating
$E_h(s_{jh}^{in}, p)$	Duty of task which needs cooling
$c_u(s_{jh}^{in}, p)$	Cooling water required by a hot task
$h_u(s_{jc}^{in}, p)$	Steam required by a cold task
$mu(s_{jc}^{in}, p)$	Amount of material processed by cold task
$mu(s_{jh}^{in}, p)$	Amount of material processed by hot task
$T^i(v, p)$	Initial temperature of a storage vessel
$T^f(v, p)$	Final temperature of a storage vessel
$T^{out}(s_{jc}^{in}, p)$	Outlet temperature of a cold task
$T^{out}(s_{jh}^{in}, p)$	Outlet temperature of a hot task
$T^{in}(s_{jc}^{in}, p)$	Inlet temperature of a cold task
$T^{in}(s_{jh}^{in}, p)$	Inlet temperature of a hot task
$t_u(s_{jc}^{in}, p)$	Time at which a cold task starts being active
$t_u(s_{jh}^{in}, p)$	Time at which a hot task starts being active
$t_p\left(s_{jc}^{in}, p\right)$	Time at which a cold task stops being active
$t_p\left(s_{jh}^{in}, p\right)$	Time at which a hot task stops being active
$t_o(s_{jc}^{in}, v, p)$	Time at which a heat storage starts being active when integrated with a cold task
$t_o(s_{jh}^{in}, v, p)$	Time at which a heat storage starts being active when integrated with a hot task
$t_f(s_{jc}^{in}, v, p)$	Time at which a heat storage stops being active when integrated with a cold task
$t_f(s_{jh}^{in}, v, p)$	Time at which a heat storage stops being active when integrated with a hot task
$qs(s_p, p)$	Amount of product at the end of the time horizon
$Qc(s_{jc}^{in}, v, p)$	Heat transferred from storage to cold task
$Q_h(s_{jh}^{in}, v, p)$	Heat transferred from hot task to storage
$Q_e(s_{jh}^{in}, s_{jc}^{in}, p)$	Amount of heat directly transferred between a hot and cold task
$W(v)$	Capacity of heat storage
$e_{sto}(v)$	Binary variable indicating the existence of a heat storage vessel
$x(s_{jc}^{in}, s_{jh}^{in}, p)$	Binary variable indicating direct integration between a hot and cold task

$y(s_{jc}^{in}, p)$ Binary variable indicating an active cold task
$y(s_{jh}^{in}, p)$ Binary variable indicating an active hot task
$z(s_{jc}^{in}, v, p))$ Binary variable indicating an active heat storage vessel integrated with a cold task
$z(s_{jh}^{in}, v, p))$ Binary variable indicating an active heat storage vessel integrated with a hot task

Parameters

α_{sto} Fixed cost of heat storage vessel
β_{sto} Variable cost of heat storage vessel
$\alpha(s_j^{in})$ Coefficient of constant term for processing time of a task
$\beta(s_j^{in})$ Coefficient of variable term for processing time of a task
A^F Annualizing factor
a Annual fractional discount factor
θ Cost function exponent
$c_p(s_{jc}^{in})$ Specific heat capacity of a cold task
$c_p(s_{jh}^{in})$ Specific heat capacity of a hot task
C_p^w Specific heat capacity of heat transfer medium
cu_c Cost of cold utility
hu_c Cost of hot utility
hr/yr Amount of hours the plant operates per year
H Time horizon of interest
M Any large number
n Lifespan of heat storage vessels in years
$SP(s_p)$ Selling price of products
$T^s(s_{jh}^{in})$ Inlet temperature of a hot task
$T^s(s_{jc}^{in})$ Inlet temperature of a cold task
$T^t(s_{jh}^{in})$ Outlet temperature of hot task
$T^t(s_{jc}^{in})$ Outlet temperature of a cold task
T^L Lower bound for initial temperature of a heat storage vessel
T^U Upper bound for initial temperature of a heat storage vessel
ΔT^L Minimum allowable temperature difference
W^L Lower bound for size of a heat storage vessel
W^U Upper bound for size of a heat storage vessel
Q_e^L Lower bound for amount of heat transferred between two tasks
Q_e^U Upper bound for amount of heat transferred between two tasks

1 Introduction

The use of batch chemical processes has gained popularity globally, due to their use in the production of low volume and high value products in the pharmaceutical, food, explosives, and speciality chemical industries [26]. Due to the escalating growth in the utilisation of batch chemical processes, research and development within the field has been intensified in order to develop optimisation techniques that can be used to operate the processes at optimal conditions. In the past the focus has been on design methods that are aimed at minimising the capital investment based on the selection of capital equipment. The focus has since shifted to optimisation methods that lead to a reduction in operating costs, such as utility costs by reducing the energy requirement in the process [5]. Direct and indirect heat integration can be used to minimise energy in batch processes. Direct heat integration is applied when a hot stream and a cold stream exchange heat with each other and indirect heat integration refers to heat/energy savings via a dedicated heat storage facility for later use. There are two main ways in which energy minimisation in batch plants has been studied, namely; the graphical optimisation methods, where the schedule is predetermined, and mathematical modelling optimisation methods. Some heuristics methods, where the schedule is also predetermined, have also been developed in minimising energy.

1.1 Graphical and Algebraic Techniques

Energy minimisation in batch plants was first conducted through the use of graphical techniques. There are two main methods which are used in the graphical techniques, i.e. the time average model as well as the time slice model. The time average model was first introduced by Clayton [11] where the energy of each stream was averaged over the batch cycle time. The minimum external utility requirement was then determined by taking into account the heat exchanged internally between streams. This method does not consider the discontinuous existence of streams which results in an overestimation of energy exchanged between streams.

The second method is the time slice model. This method uses the schedule of the batch process and divides the starting and ending times of tasks into slices or intervals. Each interval is then observed as a continuous process. The pinch point of every interval is then obtained in a similar manner like that in continuous processes. This method was first introduced by Obeng and Ashton [23]. The vast majority of energy minimisation techniques in the last three decades constituted of mainly graphical techniques [16, 17, 29] and were continuously explored in the 21th century [13].

Recent work in energy minimisation through graphical techniques includes the work of Yang et al. [30] which uses the Pseudo-T-H diagram (PTHDA) and the time slice model. The model applies both direct and indirect heat integration with the objective of minimising the total annual cost (TAC). Anastasovski [2] presented work that aims to design a common heat exchanger network for batch operations with the use of the time slice model. Chaturvedi and Bandyopadhyay [7] proposed a methodology aimed at overcoming the limitations that occur when using Time–Dependent Heat Cascade Analysis (TDHCA). The novelty of the methodology proposed by Chaturvedi et al. [8] is the shifting or delaying of product streams, in order for the product streams to be integrated with available cold/hot stream later in the time horizon.

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

1.2 Mathematical Modelling Techniques

Time can be captured in its exact form through the use of mathematical modelling as demonstrated by Papageourgiou et al. [24] through the study that involved direct and indirect heat integration in batch plants. In the formulation, indirect heat integration made use of a heat transfer medium (HTM) which acted as a mechanism for transferring heat from one operation to another as well as for storing energy over time. Bozan et al. [6] presented a study in which scheduling as well as utility usage was considered. An integrated approach was developed which included a simple synthesis algorithm and a nonlinear model. Barbosa-Povoa et al. [4] presented a methodology based on the work of Barbosa-Povoa and Macchietto [3] which was aimed at designing a batch process plant that considered the operation of the plant as well as the energy requirements.

A methodology which only considered indirect heat integration was presented by Chen and Ciou [10]. Due to the fact that a predetermined schedule of the process was used which only considered the production of one overall batch in which each task only occurred once in the time horizon, the possibility of direct heat integration was not explored. Chen and Chang [9] proposed a different technique from that of Chen and Ciou [10]. The technique was aimed at incorporating direct heat integration through the basis of resource task network scheduling which was executed simultaneously [9]. The formulation was a more general formulation in terms of the heat integration part of the model originally proposed by Majozi [20].

Moreover, Stamp and Majozi [27] presented a formulation that optimised the schedule together with the direct and indirect heat integration, as well as optimised the capacity and initial temperature of the heat storage vessel. Although heat losses of the storage vessel were taken into account in the mathematical formulation, which had previously not been done by Majozi [21], the capital cost of the heat storage vessel was not considered. The work reported by Seid and Majozi [25] introduced the ability for a task to be integrated with more than one task at a specific time interval. The heat integration framework was based on a robust scheduling formulation [26].

1.3 Heuristics and Hybrid Methods

Research in energy minimisation has also been conducted through the use of heuristics as well as a combination of the above mentioned techniques.

The seminal work done on heat integration in batch plants was by Vaselenak et al. [28] which made use of heuristics. The approach used temperature profiles and the heuristic approach as well as a mixed integer linear programming model to determine the optimal heat integration of batch plants. De Boer et al. [12] presented a case study which was performed on a process from the Dutch chemical company Dr. W. Kolb BV for the evaluation of high temperature storage units. Holczinger et al. [15] presented a study based on the S-graph approach proposed by Adonyi et al. [1] where it was assumed that heat exchangers are present for all hot-cold stream pairs and that each hot or cold stream is allowed to be matched with only one hot or cold stream. The aim of this work is an extension of the work proposed by Adonyi et al. [1] by allowing the streams to have heat exchanges with multiple other streams and takes into account the limitation on the number of available heat exchangers and their scheduling.

In this chapter, mathematical optimisation is used to optimise the schedule of batch processes together with energy requirement of the plant. Most of the work done on heat integration either focuses on direct heat integration or indirect heat integration. The schedules used in these models are, in most cases, predetermined which can lead to suboptimal results. In the proposed formulation, simultaneous optimisation of the schedule and heat integration is carried out by using the schedule as a foundation of the model and adding the heat integration techniques. The objective function of the schedule is then combined with the heat integration objective function and the two models are solved as one, as shown in Fig. 1. The chapter proposes a novel mathematical formulation based on the design of multiple heat storage vessels, where the operation of heat transfer between units and the heat storage vessels are adequately taken into account by allowing the time of heat transfer to coincide with the task duration. The proposed formulation uses a unit-specific model based on a continuous-time representation and State Sequence Network recipe representation (SSN).

2 Motivation for the Study

The objective of most mathematical models used in energy optimization of batch plants is to maximise profits by maximising throughput while minimising utility costs. The nature of batch processes makes it possible that there could

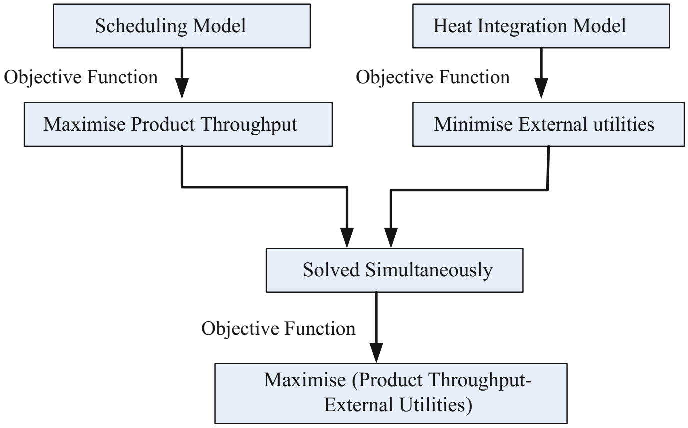

Fig. 1 Flowchart for proposed formulation

simultaneously be a task in the process that needs heating, s_{jc}^{in}, and another task that needs cooling, s_{jh}^{in}, as shown in Fig. 2a. Traditionally, this occurrence would provide an opportunity for process-process heat integration, if the thermal driving forces allow. However, if the thermal driving forces do not allow, heat storage provides another viable option towards energy minimisation. There are two scenarios that could occur, should there only be one heat storage vessel available in the plant. One of the tasks could be integrated with the heat storage vessel while the other is supplied by external utilities in order for its temperature requirement to be satisfied. This describes the first scenario depicted in Fig. 2b. The second scenario is when one task is integrated with the storage vessel while the other task is delayed for later use into the time horizon so that it could be integrated with the same heat storage vessel once the latter is available for integration, as illustrated in Fig. 2c. Clearly, this would ultimately reduce the number of batches which could be processed within the given time horizon. This drawback could be avoided by using multiple heat storage vessels that could allow for multiple heat integration between processing tasks and heat storage units in a situation where heating and cooling are required simultaneously as aforementioned. This is shown in Fig. 2d. Almost invariably, this option would allow more batches to be produced within the time horizon of interest, whilst taking advantage of available heat in the process. Consequently, this contribution is aimed at determining the optimum number, size and thermal profiles of heat storage vessels to achieve minimum energy use in multipurpose batch plants.

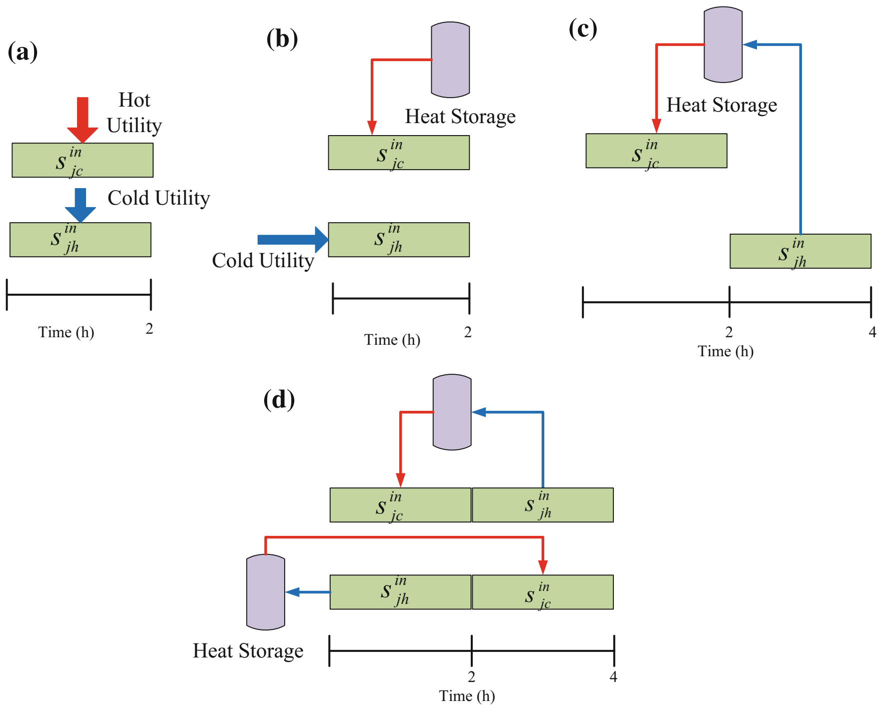

Fig. 2 **a** Tasks requiring heating/cooling, **b** one heat storage vessel, **c** one heat storage vessel and **d** multiple heat storage vessels

3 Problem Statement and Objectives

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

Given:

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

Determine:

The optimal production schedule where the objective is to maximise profit and determine the optimal number of heat storage vessels with their respective optimal sizes and initial temperatures.

4 Mathematical Formulation

The formulation is based on the superstructure depicted in Fig. 3. This shows all the possible heat integration connections in the form of direct integration, indirect integration and the use of external utilities for a hot unit J_h and a cold unit J_c.

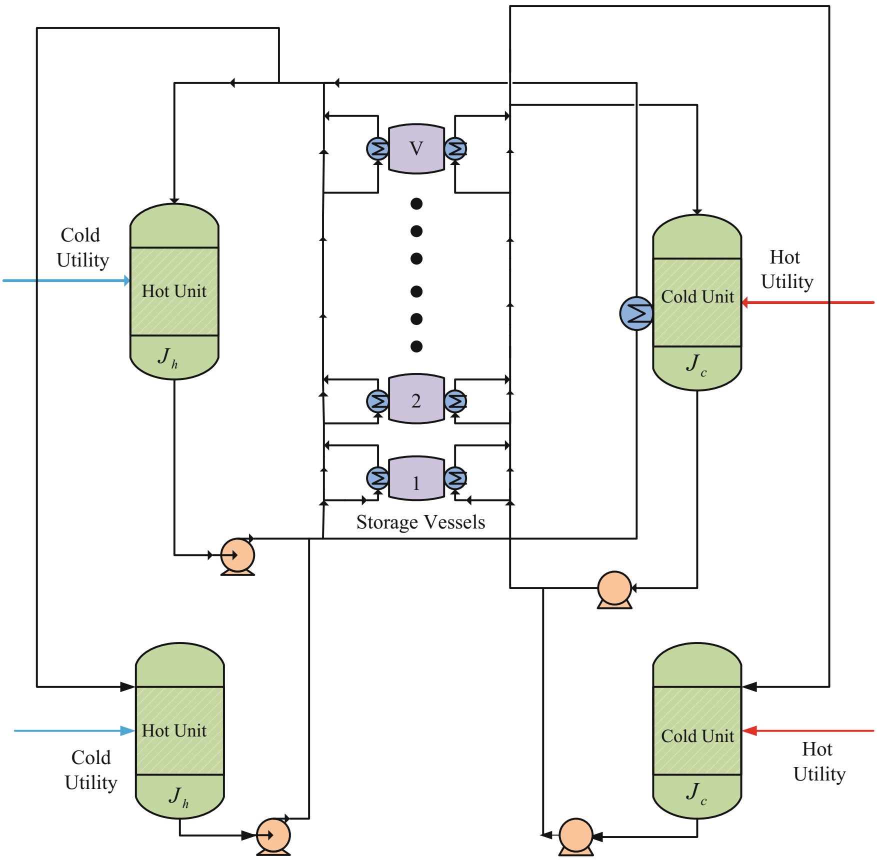

Fig. 3 General superstructure for model development

4.1 Scheduling Constraints

Scheduling constraints are critical in the mathematical formulation of batch processes. These constraints include capacity constraints of process units, duration constraints for the processing time, material balances for storage, sequence constraints, as well as allocation constraints of units. The scheduling formulation used is that of Seid and Majozi [26], which employs a unit-specific model based on a continuous-time representation.

The scheduling formulation proposed by Seid and Majozi [26] is based on finite intermediate storage which means that intermediates are stored in storage vessels of a specific size. The formulation does not take into account the transfer times of materials from one unit to another and it also does not take into account the washing or cleaning operations between tasks. Seid and Majozi [26] focused the proposed model in accurately addressing the storage constraints as well as proposing a formulation that could be solved in shorter CPU times. The proposed model allows for non-simultaneous transfer of states. Non-simultaneous transfer means that when a task requires more than one state, a state can be transferred to the unit in which it will be processed in and wait for the other state to be transferred, then only can the task begin. The model is a base scheduling model which can then be used as foundation for heat integration or water minimisation.

4.2 Allocation Constraints

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

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

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

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

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

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

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

$$\begin{gathered}\sum_{s_j^{in} \in S_{jc}^{in}} z\left(s_j^{in}, v, p\right) + \sum_{s_j^{in} \in S_{jh}^{in}} z\left(s_j^{in}, v, p\right) \leq 1 \\ \forall s_{jh}^{in} \in S_{jh}^{in}, s_{jc}^{in} \in S_{jc}^{in}, p \in P, v \in V\end{gathered} \tag{5}$$

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

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

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

4.3 Duties of Tasks and Heat Storage Vessels

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

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

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

The duties of the heating and cooling tasks are obtained by using the difference between the supply temperatures and the target temperatures of the tasks. The duties are obtained in this way because the formulation is based on variable batch size that must be taken into account in determining the duties as the duties are a function of the batch size. The cooling duty is given by constraint (10) and the heating duty is given by constraint (11). The heat capacities, $c_p\left(s_j^{in}\right)$, of the states can be found in Appendix A

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

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

4.4 Design Constraints

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

$$T^L \leq T^i(v,p) \leq T^U \quad \forall p \in P, v \in V \tag{12}$$

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

$$e_{sto}(v)W^L \leq W(v) \leq e_{sto}(v)W^U \quad \forall v \in V \tag{13}$$

4.5 Temperature Constraints

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

4.6 Utility Usage by Tasks

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

$$E_h\left(s_{jh}^{in},p\right)y\left(s_{jh}^{in},p\right) = \sum_{v} Q_h\left(s_{jh}^{in},v,p\right) + c_u\left(s_{jh}^{in},p\right) + \sum_{s_{jc}^{in}} Q_e\left(s_{jh}^{in},s_{jc}^{in},p\right)$$
$$\forall s_{jh}^{in} \in S_{jh}^{in}, \forall s_{jc}^{in} \in S_{jc}^{in}, p \in P, v \in V \tag{27}$$

$$E_c\left(s_{jc}^{in},p\right)y\left(s_{jc}^{in},p\right) = \sum_{v} Q_c\left(s_{jc}^{in},v,p\right) + h_u\left(s_{jc}^{in},p\right) + \sum_{s_{jh}^{in}} Q_e\left(s_{jh}^{in},s_{jc}^{in},p\right)$$
$$\forall s_{jh}^{in} \in S_{jh}^{in}, \forall s_{jc}^{in} \in S_{jc}^{in}, p \in P, v \in V \tag{28}$$

4.7 Limits of Heat Exchanged During Direct Heat Integration

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

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

4.8 Time Constraints

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

4.9 Objective Function

The objective of the model is to maximize profit in the batch process which consists of the revenue from the products, cost of external cold utility and hot utility defined as cu_c and hu_c, respectively, and the capital cost of the heat storage vessels which was omitted from the indirect heat integration formulation of Stamp and Majozi [27]. The cost function of the heat storage vessels is nonlinear and was obtained from the work of Li and Chang [19]. The plant is assumed to be operational for 7920 h per year while the exponent of the cost function is assumed to be 0.6. The fixed cost of a single heat storage vessel is c.u[1] 48,000 and the variable cost of a single heat storage vessel dependent on the size of the heat storage vessel is given as c.u 280,000. The objective function is given by constraint (44) and the annualizing factor is given by constraint (45) obtained from Foo [14] where the annual fractional discount factor is assumed to be 15% and lifespan of the heat storage vessels is 3 years. The cost of raw materials used in the process is not taken into account in the objective function.

[1]c.u = cost units

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

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

5 Literature Examples

The mathematical formulation was applied to two illustrative examples adapted from Majozi [22] and Kondili et al. [18]. The examples involve multipurpose batch plants which have tasks that require either heating or cooling. The models were solved in GAMS 24.3.2 using the general purpose global optimisation solver BARON in Intel® Core™ i7-3770 CPU @ 3.40 GHz, RAM 8.00 GB.

5.1 First Illustrative Example (Adapted from Majozi [22])

A batch plant which consists of two reactors, two filters and a distillation column was considered for the first example. The recipe, that is the procedure that must be followed in order to convert the raw materials to the final products, is represented as a state sequence network (SSN) in Fig. 4. SSN is a representation of the recipe as a diagram. The materials/states used in the process such as raw materials, intermediates, waste products and products that are used in the sequence and the processes/tasks which take place i.e. reaction and filtration are denoted as nodes. The mass fraction of the states used to perform a certain task is also denoted on the SSN in

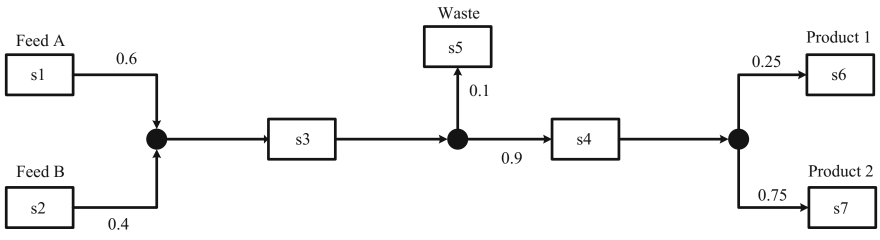

Fig. 4 SSN for first illustrative example

order to quantify the amount of state used for each task. The first illustrative example consists of three main tasks which is reaction, filtration and distillation/separation. The reaction task can take place in either reactor 1 or 2, using state 1 and 2 as raw materials to produce state 3 and needs to be cooled from 100 to 70 °C. The filtration task can be carried out in filters 1 and 2 where state 3 is filtered to obtain state 4 and state 5 which is a waste product. The separation task distils state 4 into state 6 and 7 is carried out in the distillation column and should be heated from 65 to 80 °C. Figure 5a shows the process flow diagram of the illustrative example.

The reaction task is 2 h long and a maximum batch size of 60 kg can be produced in each reactor. The filtration is 1 h long and can handle a maximum batch size of 80 kg as its feed. The distillation task is 2 h long and takes a maximum batch size of 140 kg as the feed to the distillation column. The batch plant has a tank farm where each state used or produced from the process can be stored. The maximum storage capability of the intermediate states is shown in Fig. 5b. The initial inventory of the raw materials, state 1 and 2 is given as 1000 kg each at the start of production.

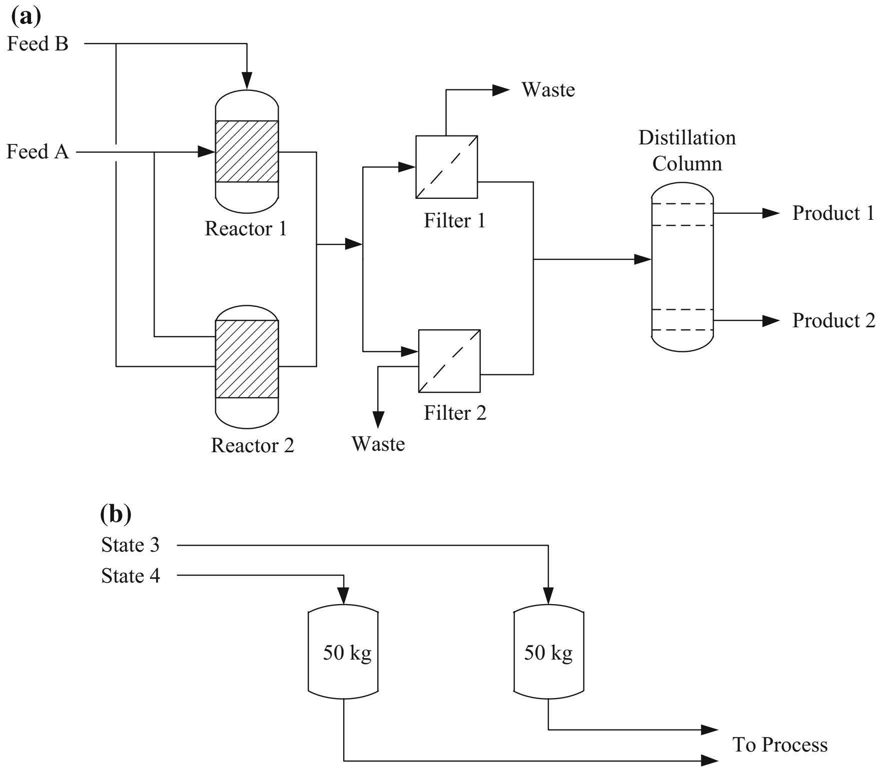

Fig. 5 **a** Process flow diagram, **b** tank farm for first illustrative example

The detailed scheduling data and the detailed heating/cooling requirement data is given in Tables 3, 4 and 5, and the detailed heat storage vessel cost function parameters are given in Table 6 in Appendix A. The superstructure of the example is given in Fig. 6. The superstructure had a maximum of four heat storage vessels which could be used for indirect heat integration together with opportunities for direct heat integration and the use of external utilities.

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

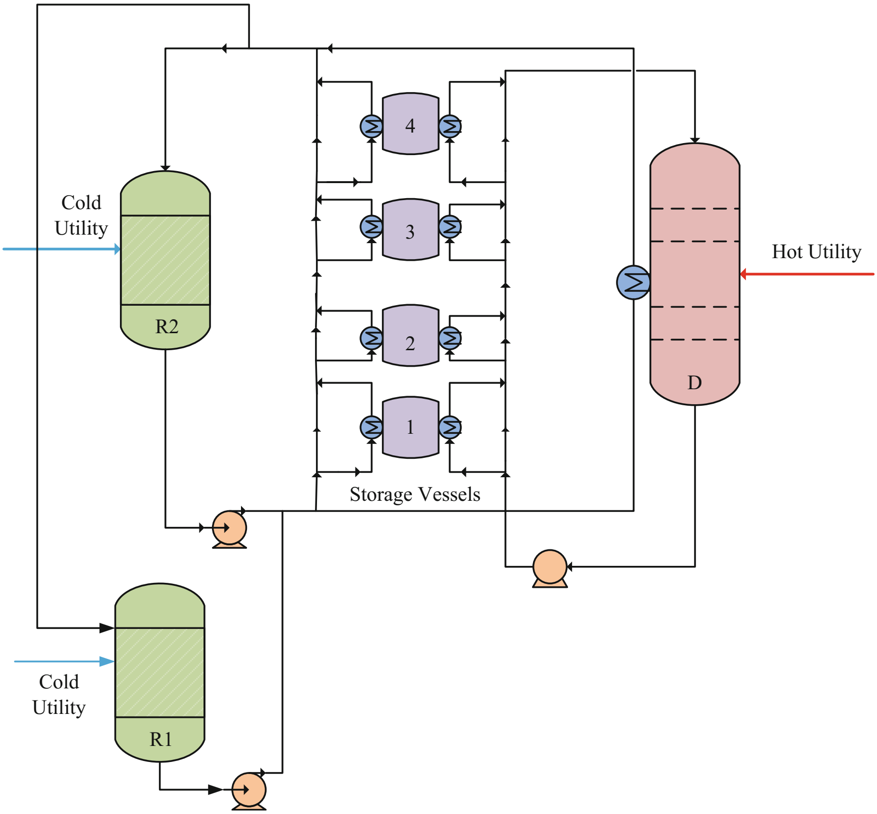

Fig. 6 Superstructure for first illustrative example

5.1.1 Results and Discussion

The results obtained from the application of the model are given in Table 1. The objective value obtained for scenario 1 was c.u 31.4×10^6. This is mainly due to the fact that only three main tasks take place in the process. Two of those tasks require heating/cooling and as such a huge amount of external utilities is used for the first scenario. Scenario 2 resulted in an objective value of c.u 33.5×10^6. The hot utility was eliminated and the cold utility requirement was 50.40 MJ. Scenario 3 resulted in an objective value of c.u 34.1×10^6 and no external utilities requirements.

The proposed mathematical formulation resulted in an optimal number of three heat storage vessels which are depicted in the resultant flowsheet in Fig. 7. The flowsheet shows that the model achieves its optimal objective value only when indirect heat integration occurs. It should be noted that 100% decrease of external utilities does not take into account the cold and hot utilities that are used in the heat storage vessels to achieve the initial temperatures although the cost of the heat transfer medium is taken into account with the cost of storage. The objective value of the scheduling model, where no utilities are considered, was found to be c.u 34.2×10^6 and scenario 3 (multiple heat storage vessels model) resulted in an objective of c.u 34.1×10^6. It can be seen that the multiple heat storage vessels model achieved an objective value closest to the scheduling model objective value, as compared to scenario 1 and 2. This shows that the proposed mathematical formulation not only minimises the use of external utilities, but also allows for flexibility with regards to time. This means that more batches can be produced within the time horizon as though utilities were not considered like in the scheduling model. The objective value of the proposed model is however not equal to the scheduling objective value because the capital costs of the heat storage vessels were accounted for in the objective function of multiple heat storage vessels model, whereas the scheduling model takes into account the amount of product with its selling price only.

Table 1 Results for first illustrative example

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

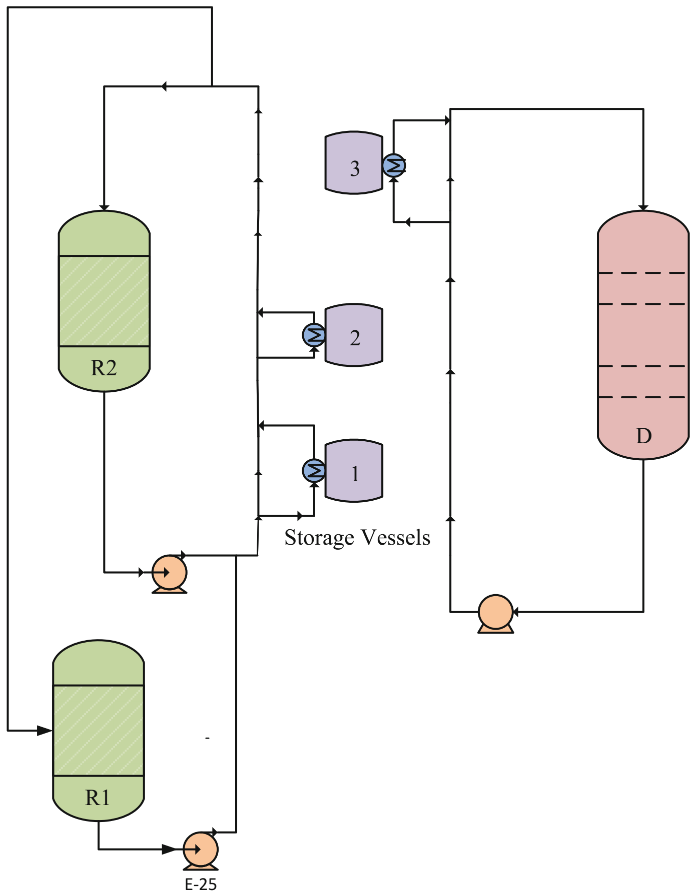

Fig. 7 Resultant flowsheet for first illustrative example

It is evident that the heat integration configuration of the heat storage vessels resulted in one heat storage being used to heat the distillation task, while the other two heat storage vessels were used to cool down the reaction task in both reactors as illustrated in the Gantt chart in Fig. 8. For this specific example, the configuration of using all heat storage vessels as both sinks and sources was not the best solution. This can be attributed to the fact that there were only two tasks which required external utilities, therefore segregating the usage of heat storage vessels to suit the needs of the tasks resulted in a simpler heat exchange configuration. The initial temperatures of the heat storage vessels also affect the type of configuration output.

The heat storage vessels had initial temperatures of 20, 20 and 160 °C and sizes of 112.5, 150 and 116.2 kg, respectively. The temperature profiles of the heat storage vessels are depicted in Fig. 9 which show the changes in temperature of each of the heat storage vessels throughout the time horizon. The heat loss of the

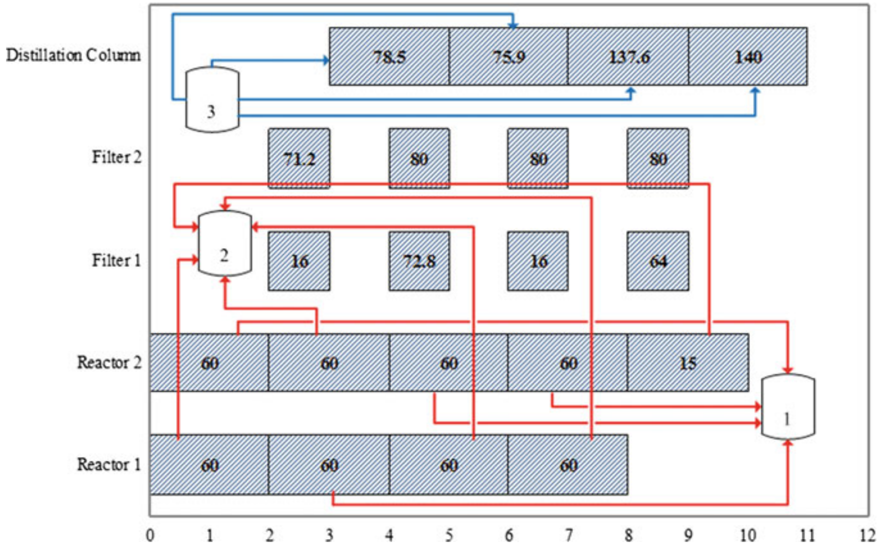

Fig. 8 Gantt chart using proposed model for first illustrative example

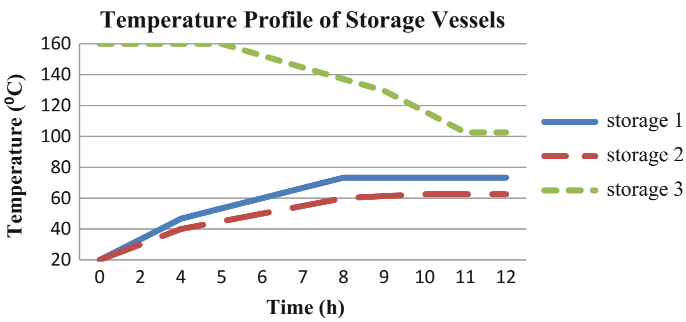

Fig. 9 Temperature profile for heat storage vessels for first illustrative example

heat storage vessels was not considered due to the short length of the time horizon. Due to the nonlinear nature of the model and the computational intensity required in solving it, the CPU time was set at a limit of 6000 s for the single heat storage vessel and the multiple heat storage vessel scenarios. Given that the problem being solved is a design problem a longer CPU time can be tolerated.

Piping costs were not taken into account in the mathematical formulation. Figure 10 shows the configuration of a unit with the heat exchanger used to facilitate heat transfer. The unit will have standard piping whether the heat transfer medium is from external utilities, direct or indirect heat integration. The additional piping costs will come from each heat storage vessel added to the heat transfer

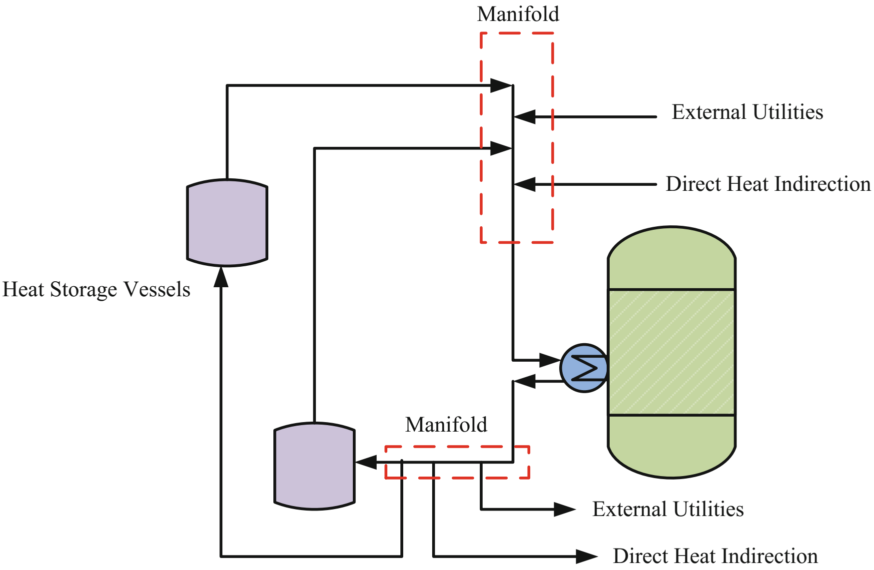

Fig. 10 Piping design of a heat storage vessel

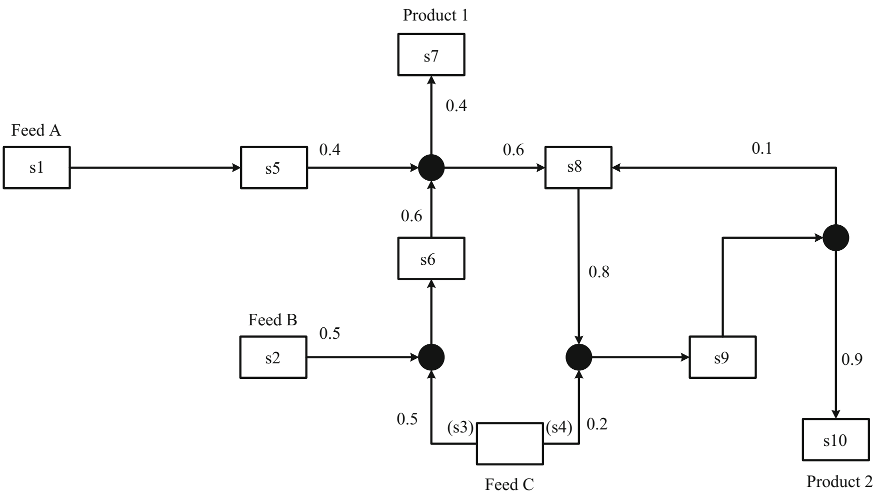

Fig. 11 SSN for second illustrative example

configuration through indirect heat integration as shown in Fig. 10. The total cost of piping can then be minimised by optimally arranging the configuration of the heat storage vessels and the units.

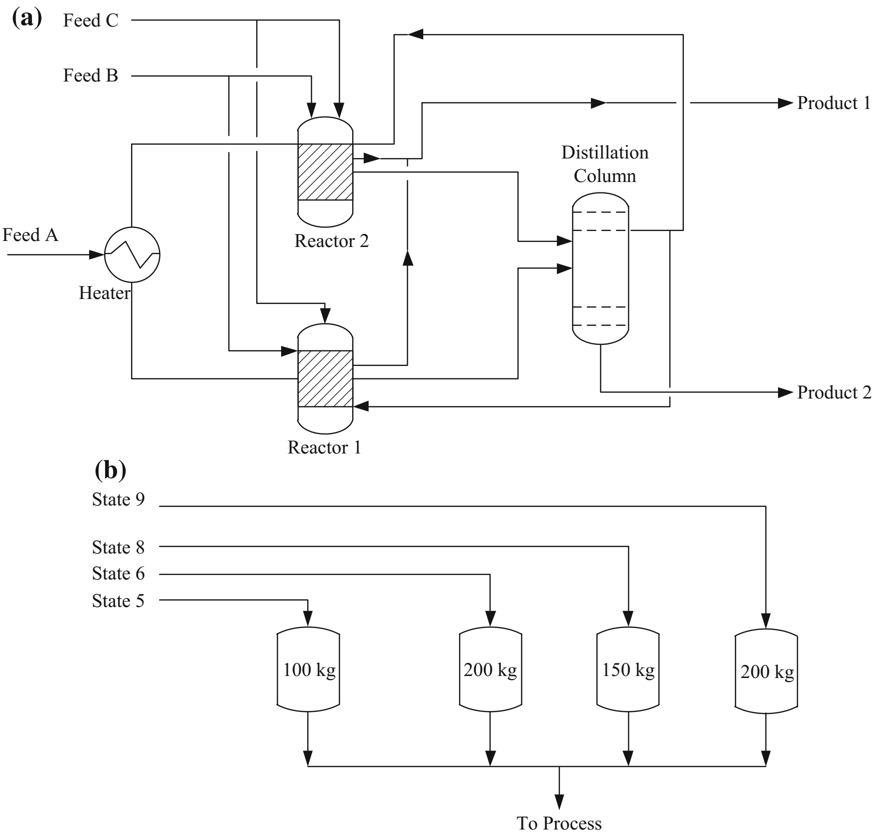

Fig. 12 **a** Process flow diagram, **b** tank farm for second illustrative example

5.2 Second Illustrative Example (Adapted from Kondili et al. [18])

A multipurpose batch plant which consists of a heater, two reactors, in which three reactions can occur and a separation unit was also considered. The recipe is represented as a State Sequence Network (SSN) in Fig. 11 which shows the procedural steps of the process. The SSN is represented in the same way as in the first illustrative example. The second illustrative example consists of heating, three reaction steps and separation. The heat task heats state 1 to produce state 5. Reaction 1 task reacts state 2 and 3 to produce state 6 and must be cooled from 100 to 70 °C. Reaction 2 reacts state 5 and 6 to produce state 7, which is product 1 and state 8 and must be heated from 70 to 100 °C. Reaction 3 reacts state 4 and 8 to produce state 9 and must be cooled from 130 to 100 °C. The separation task separates state 9 into state 10, which is product 2, and state 8 which is recycled back

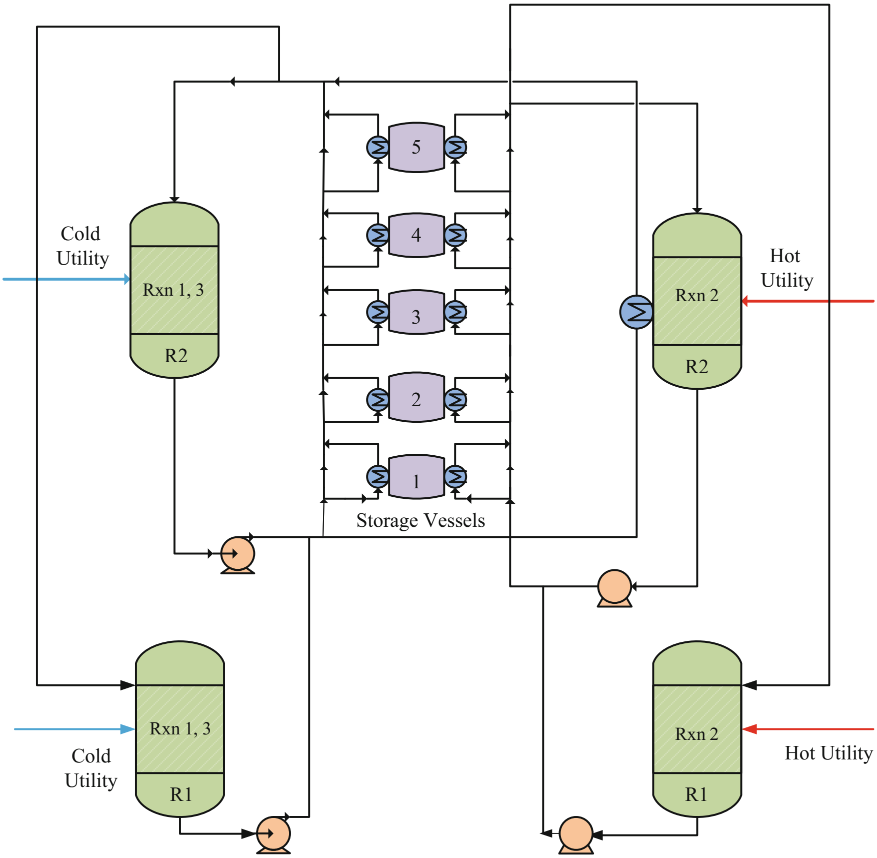

Fig. 13 Superstructure for second illustrative example

to be used for reaction 3. Figure 12a shows the process flow diagram of the illustrative example.

The duration of all tasks varies depending on the quantity of the batch being processed or produced. The constants used to determine the duration of the batches can be found in Appendix A. The maximum batch size that can be heated for the heating task is 100 kg. The maximum batch size to be produced in reactors 1 and 2 is 50 and 80 kg, respectively. The separation can handle a maximum of 200 kg of feed to be separated. The tank farm which shows the maximum storage capability of the intermediate states is shown in Fig. 12b. The initial inventory of the raw materials, states 1, 2, 3 and 4 is given as 1000 kg each at the start of production.

The detailed scheduling data and the detailed heating/cooling requirement data is given in Tables 7, 8 and 9, and the detailed heat storage vessel cost function parameters are given in Table 10 in Appendix A. The three scenarios considered for the first example were once again considered for the second example namely; base case scenario (scenario 1), one heat storage vessel (scenario 2) as well as multiple heat storage vessels (scenario 3). The superstructure for the example is given in Fig. 13. The superstructure had a maximum of five heat storage vessels which could be used for indirect heat integration together with opportunities for direct heat integration and the use of external utilities. The selling price for products 1 and 2 is c.u 20 and the cost of the cold and hot utilities is c.u 0.02 and c.u 1, respectively.

5.2.1 Results and Discussion

The resultant flowsheet and the Gantt chart with the heat integration configuration are presented in Figs. 14 and 15, respectively. Scenario 1 resulted in an objective value of c.u 465.2×10^3, hot utility requirement of 16.6 MJ and cold utility requirement of 21 MJ for a 10 h time horizon. Scenario 2 resulted in an increased objective value of c.u 2.5×10^6 and a cold utility of 15.6 MJ. A further increase in

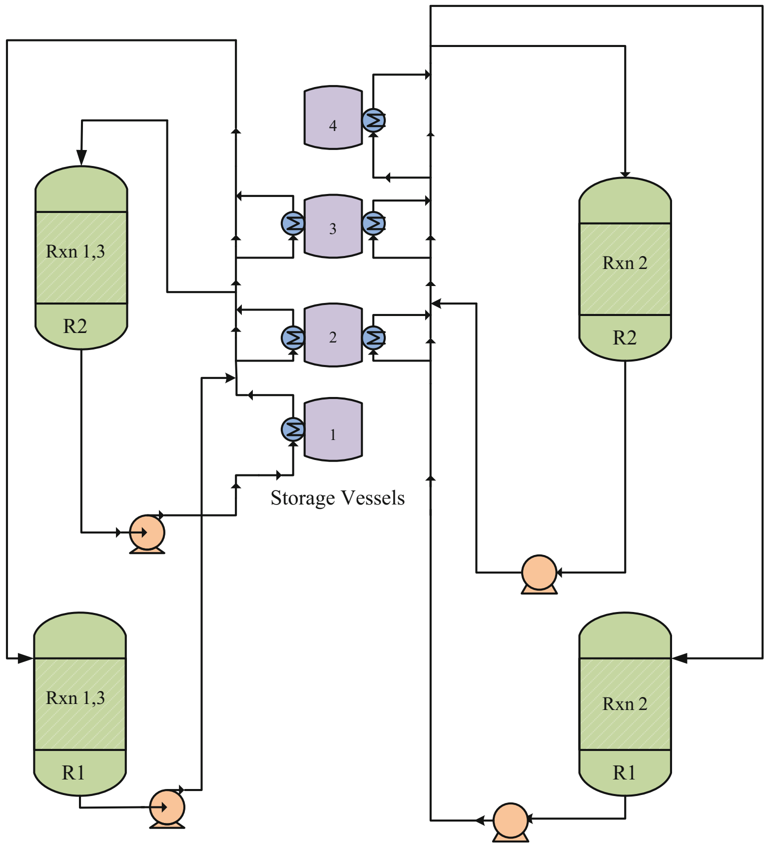

Fig. 14 Resultant flowsheet for second illustrative example

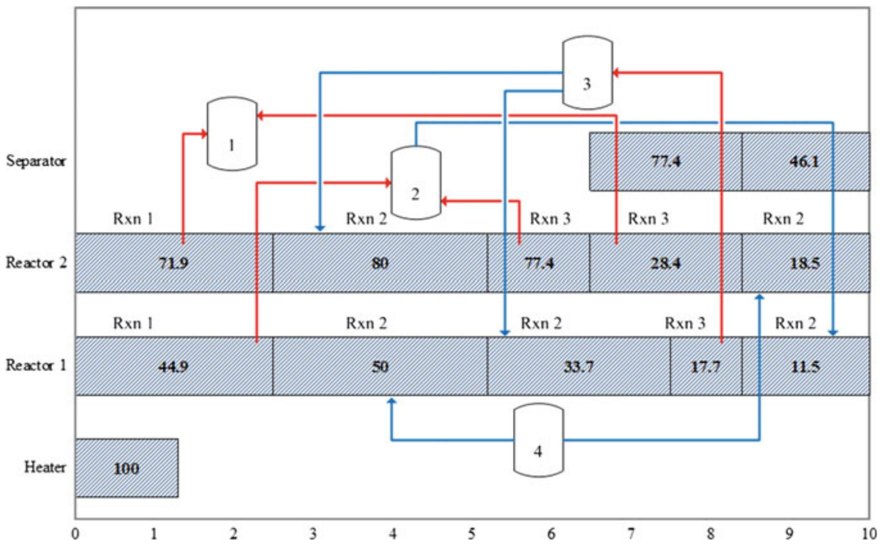

Fig. 15 Gantt chart using proposed model for second illustrative example

the objective value (c.u 2.9×10^6) was achieved for scenario 3. No external utilities were used when the proposed model was applied to the illustrative example. This demonstrates that the application of multiple heat storage results not only in the decrease of operational costs, in this instance external utilities, but can result in flexibility of time in the plant which will ultimately affect the revenue of the plant. There is trade-off between cost of the heat storage vessels and minimisation of energy using indirect heat integration. The results of the proposed model show that high savings in external utilities can still be achieved even with the consideration of the capital cost of the storage vessels. The results for the proposed formulation are given in Table 2.

Table 2 Results for second illustrative example

	No integration	One heat storage vessel	Multiple heat storage vessels
Objective (c.u)	465.2×10^3	2.5×10^6	2.9×10^6
Cold utility (MJ)	21.0	15.6	0
Hot utility (MJ)	16.6	0	0
Discrete variables	72	143	236
Continuous variables	337	639	1035
Time points	5	5	5
CPU time (s)	3	6000	6000

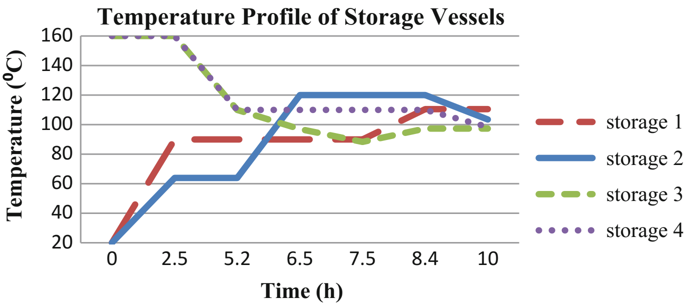

Fig. 16 Temperature profile of heat storage vessels for second illustrative example

The proposed model achieved an optimal number of four heat storage vessels together with the optimal sizes of 25.7, 25.6, 36.6 and 22.9 kg respectively. The optimal initial temperatures of the vessels were 20, 20, 160 and 160 °C respectively. The temperature profiles of the heat storage vessels for the 10 h time horizon are depicted in Fig. 16.

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

6 Conclusion

A mathematical formulation for direct and indirect heat integration with multiple heat storage vessels has been developed and applied to two case studies. The emphasis of the formulation is the use of multiple heat storage vessels by looking at the design of the heat storage vessels as well as the synthesis of the heat exchanger network of the batch process. The formulation is aimed at maximising profit in the plant while taking into account the utility and capital costs of the heat storage vessels as well as determining the size and initial temperatures of the heat storage vessels. The application of the formulation results in an increase in profit and the elimination of external utilities use in the plant. The first illustrative example resulted in a 100% decrease of external utilities and an 8.88% increase in profit was obtained when multiple heat storage vessels were considered as compared to when no heat integration is applied to the illustrative example. The second illustrative example resulted in a 100% decrease in external utilities as well as a 17.74%

increase in profit when multiple heat storage vessels were considered as compared to a scenario where only one heat storage vessel is available in the plant. The total reduction in external utilities used in both examples does not include the hot and cold utilities used in the heat storage vessels as heat transfer mediums which are already available at the beginning of the time horizon. The use of multiple heat storage vessels showed a resultant flexibility in time which maximised the throughput of the plant while minimising the operational costs of the plant.

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Appendix A

The scheduling data for the first illustrative example is given in Table 3. The table shows each task with the corresponding maximum batch size and the residence time.

Additional scheduling data is given in Table 4. This table shows each state with the corresponding initial inventory values, maximum storage and the revenue or cost of each state. As previously mentioned, the cost of raw materials is assumed to be zero.

Table 3 Scheduling data for first illustrative example

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

Table 4 Scheduling data for first illustrative example

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

The heat integration data is given in Table 5. This table gives the supply and target temperatures for each task as well as the specific heat capacities.

The heat storage vessels cost function parameters are given in Table 6. These parameters are the fixed cost, variable cost, operational time, cost function exponent and the number of years a heat storage vessel can be used.

The scheduling data for the first illustrative example is given in Table 7. The table shows each task with the corresponding maximum batch size and the residence time.

Additional scheduling data is given in Table 8. This table shows each state with the corresponding initial inventory values, maximum storage and the revenue or cost of each state. As previously mentioned, the cost of raw materials is assumed to be zero.

Table 5 Heat integration data for first illustrative example

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

Table 6 Heat storage vessel cost function parameters

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

Table 7 Scheduling data for second illustrative example

Task	Unit	Max batch size (kg)	Minimum time $\alpha\left(s_j^{in}\right)$ (hr)	Variable time $\beta\left(s_j^{in}\right)$ ($\times 10^{-3}$) (hr/kg)
Heating	1	100	0.667	6.67
Reaction 1	2	50	1.334	26.64
	3	80	1.334	16.65
Reaction 2	2	50	1.334	26.64
	3	80	1.334	16.65
Reaction 3	2	50	0.667	13.32
	3	80	0.667	8.33
Separation	4	200	1.3342	6.66

Table 8 Scheduling data for second illustrative example

State	Material state	Initial inventory (kg)	Max storage (kg)	Revenue or cost (c.u)
S1	Feed A	1000	1000	0
S2	Feed B	1000	1000	0
S3, S4	Feed C	1000	1000	0
S5	Hot A	0	100	0
S6	Int AB	0	200	0
S8	Int BC	0	150	0
S9	Impure E	0	200	0
S7	Prod 1	0	1000	20
S10	Prod 2	0	1000	20
	Cold utility			0.02
	Hot utility			1

Table 9 Heat integration data for second illustrative example

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

Table 10 Heat storage vessels cost function parameters

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

The heat integration data is given in Table 9. This table gives the supply and target temperatures for each task as well as the specific heat capacities.

The heat storage vessels cost function parameters are given in Table 10. These parameters are the fixed cost, variable cost, operational time, cost function exponent and the number of years a heat storage vessel can be used.

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