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OPTIMUM HEAT STORAGE DESIGN FOR HEAT INTEGRATED MULTIPURPOSE BATCH PLANTS

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ABSTRACT

Heat integration to minimise energy usage in multipurpose batch plants has been in published literature for more than two decades. In most present methods, time is fixed *a priori* through a known schedule, which leads to suboptimal results. The method presented in this paper treats time as a variable, thereby leading to improved results. Both direct and indirect heat integration are considered together with optimisation of heat storage size and initial temperature of heat storage medium. The resulting model exhibits 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 due to idling are also considered. This work is an extension of MILP model of Majozi [1], which was more suited to multiproduct rather than multipurpose batch facilities. 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.

INTRODUCTION

Batch processes are commonly used for the manufacture of products required in small quantities or for specialty and complex products of high value. Typical industries include food, pharmaceuticals, fine chemicals, biochemicals and agrochemicals. Approximately half of all production facilities make use of batch processes [2]. Batch operations are generally run on a smaller scale compared to continuous operations and utility requirements are therefore considered less significant. Energy consumption is commonly estimated to be about 5% to 10% of total costs [3,4,5]. Some batch industries do, however, have a much higher utility requirement than others. For example, utility requirements in the food industry, breweries, dairies, meat processing facilities, biochemical plants and agrochemical facilities contribute largely to the total cost [6,7,8,9,10,11,12,1]. Although the energy savings obtainable through heat integration may not be as large in magnitude as in the continuous case, energy savings have often been neglected in batch processes in the past and large percentage savings are possible.

NOMENCLATURE

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

$A_1(u)$	[m^2]	area for convective heat transfer from heat transfer medium
$A_3(u)$	[m^2]	area for convective heat transfer to environment
$cw(s_{in,j_h}, p)$	[kWh]	external cooling required by unit j_h conducting the task corresponding to state s_{in,j_h} at time point p
$L(u)$	[m]	height of heat storage vessel
$Q(s_{in,j}, u, p)$	[kWh]	heat exchanged with heat storage unit u at time point p
$\dot{Q}_{loss}(u, p)$	[kW]	rate of heat loss from idle heat storage unit
$R_{conv_1}(u)$	[ºC/kW]	convective resistance of heat transfer medium
$R_{conv_3}(u)$	[ºC/kW]	convective resistance of ambient air
$R_{ins}(u)$	[ºC/kW]	conductive resistance of insulation
$R_{ves}(u)$	[ºC/kW]	conductive resistance of heat storage vessel
$R_{tot}(u)$	[ºC/kW]	thermal resistance for heat storage unit
$st(s_{in,j_c}, p)$	[kWh]	external heating required by unit j_c conducting the task corresponding to state s_{in,j_c} at time point p
$\Delta\dot{T}(u, p)$	[ºC/h]	rate of temperature drop in heat storage unit u due to heat losses
$T_{\infty_{in}}(u, p)$	[ºC]	steady state temperature equal to the final temperature in the heat storage vessel, $T_f(u, p)$
$T_0(u, p)$	[ºC]	initial temperature in heat storage unit u at time point p
$T_f(u, p)$	[ºC]	final temperature in heat storage unit u at time point p
$\Delta t(p)$	[h]	time interval over which heat loss takes place
$t_0(s_{in,j}, u, p)$	[h]	time at which heat storage unit commences activity
$t_f(s_{in,j}, u, p)$	[h]	time at which heat storage unit ends activity
$t_u(s_{in,j}, p)$	[h]	time at which a stream enters unit j
$V(u)$	[m^3]	volume of heat storage unit u
$W(u)$	[ton]	capacity of heat storage unit u
$\Gamma(s_{in,j}, u, p)$	[ºC]	Glover Transformation variable
$\Psi(s_{in,j}, u, p)$	[m]	Reformulation-Linearisation variable

Binary variables

$x(s_{in,j_c}, s_{in,j_h}, p)$	[0;1]	$1 \leftarrow$ if unit j_c conducting the task corresponding to state s_{in,j_c} is integrated with unit j_h conducting the task corresponding to state s_{in,j_h} at time point p $0 \leftarrow$ otherwise
$y(s_{in,j}, p)$	[0;1]	$1 \leftarrow$ if state s is used in unit j at time point p $0 \leftarrow$ otherwise
$z(s_{in,j}, u, p)$	[0;1]	$1 \leftarrow$ if unit j conducting the task corresponding to state $s_{in,j}$ is integrated with storage unit u at time point p $0 \leftarrow$ otherwise

Parameters

c_p	[kJ/kgºC]	specific heat capacity of heat storage fluid
$E(s_{in,j})$	[kWh]	amount of heat required by or removed from unit j conducting the task corresponding to state $s_{in,j}$
h_1	[kW/m^{2}ºC]	convective heat transfer coefficient for free convection of liquids
h_3	[kW/m^{2}ºC]	convective heat transfer coefficient for free convection of gases
k_{ins}	[kW/mºC]	thermal conductivity of insulation
k_{ves}	[kW/mºC]	thermal conductivity of heat storage vessel
M	[-]	any large number
r_1	[m]	inside radius of heat storage vessel
r_2	[m]	outside radius of heat storage vessel
r_3	[m]	outside radius of insulation
$T(s_{in,j})$	[ºC]	operating temperature for processing unit j conducting the task corresponding to state $s_{in,j}$
T^L	[ºC]	lower bound for heat storage temperature
T^U	[ºC]	upper bound for heat storage temperature
$\Delta T^{\min}$	[ºC]	minimum allowable thermal driving force
$T_{\infty_{out}}$	[ºC]	steady state ambient temperature
$\tau(s_{in,j})$	[h]	duration of the task corresponding to state $s_{in,j}$ conducted in unit j
W^L	[ton]	lower bound for heat storage capacity
W^U	[ton]	upper bound for heat storage capacity

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) Costs 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.

MATHEMATICAL MODEL

The model is based on the superstructure in Figure 1.

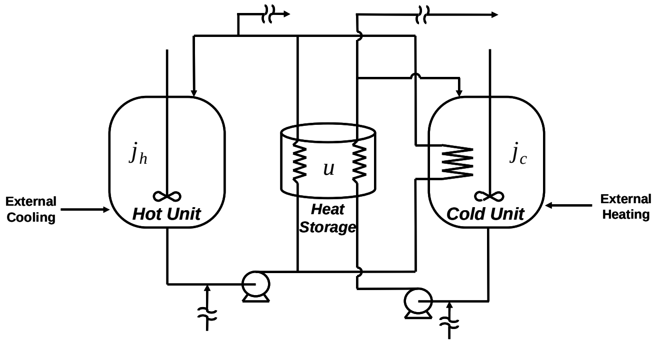

Figure 1 Superstructure for mathematical model

In addition to the necessary short term scheduling constraints [13], Constraints (1) to (22) constitute the heat integration model, useful for multipurpose batch processes with fixed batch sizes. Both direct and indirect heat integration are considered. The formulation is based on previous models in the literature [14,1]. These models could not adequately address multipurpose facilities, but were ideal for multiproduct cases.

Constraints (1) and (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.

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

$$\sum_{s_{in,j_h}} x\left(s_{in,j_c}, s_{in,j_h}, p\right) \le y\left(s_{in,j_c}, p\right),$$
$$\forall\ p \in P,\quad s_{in,j_c} \in S_{in,j} \qquad (2)$$

Constraint (3) ensures that only one hot or cold unit is heat integrated with one heat storage unit at any point in time.

$$\sum_{s_{in,j_c}} z\left(s_{in,j_c}, u, p\right) + \sum_{s_{in,j_h}} z\left(s_{in,j_h}, u, p\right) \le 1,$$
$$\forall\ p \in P,\quad u \in U \qquad (3)$$

Constraints (4) and (5) ensure that a unit cannot simultaneously undergo direct and indirect heat integration. This condition simplifies the operation of the process.

$$\sum_{s_{in,j_h}} x\left(s_{in,j_c}, s_{in,j_h}, p\right) + z\left(s_{in,j_c}, u, p\right) \le 1,$$
$$\forall\ p \in P,\quad s_{in,j_c} \in S_{in,j},\quad u \in U \qquad (4)$$

$$\sum_{s_{in,j_c}} x\left(s_{in,j_c}, s_{in,j_h}, p\right) + z\left(s_{in,j_h}, u, p\right) \le 1,$$
$$\forall\ p \in P,\quad s_{in,j_h} \in S_{in,j},\quad u \in U \qquad (5)$$

Constraints (6) and (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.

$$Q\left(s_{in,j_c}, u, p-1\right) = W(u)c_p\left(T_0(u, p-1) - T_f(u, p)\right)z\left(s_{in,j_c}, u, p-1\right),$$
$$\forall\ p \in P, p > p0,\quad s_{in,j_c} \in S_{in,j},\quad u \in U \qquad (6)$$

$$Q\left(s_{in,j_h}, u, p-1\right) = W(u)c_p\left(T_f(u, p) - T_0(u, p-1)\right)z\left(s_{in,j_h}, u, p-1\right),$$
$$\forall\ p \in P, p > p0,\quad s_{in,j_h} \in S_{in,j},\quad u \in U \qquad (7)$$

Constraint (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 $T_0(u, p0)$.

$$Q\left(s_{in,j_h}, u, p0\right) = W(u)c_p\left(T_f(u, p1) - T_0(u, p0)\right)z\left(s_{in,j_h}, u, p0\right),$$
$$\forall\ s_{in,j_h} \in S_{in,j},\quad u \in U \qquad (8)$$

Constraint (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.

$$T_0(u, p) = T_f(u, p-1),$$
$$\forall\ p \in P,\quad u \in U \qquad (9)$$

Constraints (10) and (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 $z(s_{in,j_c},u,p-1)$ or $z(s_{in,j_h},u,p-1)$ is equal to one, Constraint (10) and Constraint (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.

$$T_0(u,p-1)\le T_f(u,p)+\Delta\dot{T}(u,p-1)\Delta t(p)$$
$$+M\left(\sum_{s_{in,jc}} z(s_{in,j_c},u,p-1)+\sum_{s_{in,jh}} z(s_{in,j_h},u,p-1)\right),$$
$$\forall\ p\in P, p>p0,\quad u\in U \tag{10}$$

$$T_0(u,p-1)\ge T_f(u,p)+\Delta\dot{T}(u,p-1)\Delta t(p)$$
$$-M\left(\sum_{s_{in,jc}} z(s_{in,j_c},u,p-1)+\sum_{s_{in,jh}} z(s_{in,j_h},u,p-1)\right),$$
$$\forall\ p\in P, p>p0,\quad u\in U \tag{11}$$

Constraint (12) ensures that minimum thermal driving forces are obeyed when there is direct heat integration between a hot and a cold unit.

$$T(s_{in,j_h})-T(s_{in,j_c})\ge \Delta T^{\min}-M\left(1-x(s_{in,j_c},s_{in,j_h},p-1)\right),$$
$$\forall\ p\in P, p>p0,\quad s_{in,j_c},s_{in,j_h}\in S_{in,j} \tag{12}$$

Constraints (13) and (14) ensure that minimum thermal driving forces are obeyed when there is heat integration with the heat storage unit. Constraint (13) applies for heat integration between heat storage and a heat sink, while constraint (14) applies for heat integration between heat storage and a heat source.

$$T_f(u,p)-T(s_{in,j_c})\ge \Delta T^{\min}-M\left(1-z(s_{in,j_c},u,p-1)\right),$$
$$\forall\ p\in P, p>p0,\quad s_{in,j_c}\in S_{in,j},\quad u\in U \tag{13}$$

$$T(s_{in,j_h})-T_f(u,p)\ge \Delta T^{\min}-M\left(1-z(s_{in,j_h},u,p-1)\right),$$
$$\forall\ p\in P, p>p0,\ s_{in,j_h}\in S_{in,j},\quad u\in U \tag{14}$$

Constraint (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.

$$E(s_{in,j_h})y(s_{in,j_h},p)=Q(s_{in,j_h},u,p)+cw(s_{in,j_h},p)$$
$$+\sum_{s_{in,jc}}\min_{s_{in_{jc}},\,s_{in,jh}}\left\{E(s_{in,j_c}),E(s_{in,j_h})\right\}x(s_{in,j_c},s_{in,j_h},p),$$
$$\forall\ p\in P,\quad s_{in,j_h}\in S_{in,j},\quad u\in U \tag{15}$$

Constraint (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.

$$E(s_{in,j_c})y(s_{in,j_c},p)=Q(s_{in,j_c},u,p)+st(s_{in,j_c},p)$$
$$+\sum_{s_{in,jh}}\min_{s_{in,jc},\,s_{in,jh}}\left\{E(s_{in,j_c}),E(s_{in,j_h})\right\}x(s_{in,j_c},s_{in,j_h},p),$$
$$\forall\ p\in P,\quad s_{in,j_c}\in S_{in,j},\quad u\in U \tag{16}$$

Constraints (17) and (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.

$$t_u(s_{in,j_h},p)\ge t_u(s_{in,j_c},p)-M\left(1-x(s_{in,j_c},s_{in,j_h},p)\right)$$
$$\forall\ p\in P,\quad s_{in,j_c},s_{in,j_h}\in S_{in,j} \tag{17}$$

$$t_u(s_{in,j_h},p)\le t_u(s_{in,j_c},p)+M\left(1-x(s_{in,j_c},s_{in,j_h},p)\right)$$
$$\forall\ p\in P,\quad s_{in,j_c},s_{in,j_h}\in S_{in,j} \tag{18}$$

Constraints (19) and (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.

$$t_u(s_{in,j},p)\ge t_0(s_{in,j},u,p)-M\left(y(s_{in,j},p)-z(s_{in,j},u,p)\right)$$
$$\forall\ p\in P,\quad u\in U,\quad s_{in,j}\in S_{in,j} \tag{19}$$

$$t_u(s_{in,j},p)\le t_0(s_{in,j},u,p)+M\left(y(s_{in,j},p)-z(s_{in,j},u,p)\right)$$
$$\forall\ p\in P,\quad u\in U,\quad s_{in,j}\in S_{in,j} \tag{20}$$

Constraints (21) and (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.

$$t_u(s_{in,j},p-1)+\tau(s_{in,j})y(s_{in,j},p-1)\ge t_f(s_{in,j},u,p)$$
$$-M\left(y(s_{in,j},p-1)-z(s_{in,j},u,p-1)\right)$$
$$\forall\ p\in P, p>p0,\quad u\in U,\quad s_{in,j}\in S_{in,j} \tag{21}$$

$$t_u(s_{in,j},p-1)+\tau(s_{in,j})y(s_{in,j},p-1)\le t_f(s_{in,j},u,p)$$
$$+M\left(y(s_{in,j},p-1)-z(s_{in,j},u,p-1)\right)$$
$$\forall\ p\in P, p>p0,\quad u\in U,\quad s_{in,j}\in S_{in,j} \tag{22}$$

Constraints (6), (7) and (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 [15]. This is an exact linearisation technique and as such will not compromise the accuracy of the model. The transformation procedure for Constraint (7) leads to Constraint (23).

$$Q\left(s_{in,j_h},u,p-1\right)=W(u)c_p\left(\Gamma_1\left(s_{in,j_h},u,p\right)-\Gamma_2\left(s_{in,j_h},u,p-1\right)\right),\quad \forall\ p\in P, p>p0,\quad s_{in,j_h}\in S_{in,j},\quad u\in U \qquad (23)$$

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 [16] as discussed by Quesada and Grossmann [17]. This is demonstrated for Constraint (23), resulting in Constraints (24) to (30).

Let

$$W(u)\Gamma_1\left(s_{in,j_h},u,p\right)=\Psi_1\left(s_{in,j_h},u,p\right) \qquad (24)$$

With lower and upper heat storage capacity and temperature bounds known

$$W^L\le W(u)\le W^U \qquad (25)$$

$$T^L\le \Gamma_1\left(s_{in,j_h},u,p\right)\le T^U \qquad (26)$$

Then

$$\Psi_1\left(s_{in,j_h},u,p\right)\ge W^L\Gamma_1\left(s_{in,j_h},u,p\right)+T^LW(u)-W^LT^L \qquad (27)$$

$$\Psi_1\left(s_{in,j_h},u,p\right)\ge W^U\Gamma_1\left(s_{in,j_h},u,p\right)+T^UW(u)-W^UT^U \qquad (28)$$

$$\Psi_1\left(s_{in,j_h},u,p\right)\le W^U\Gamma_1\left(s_{in,j_h},u,p\right)+T^LW(u)-W^UT^L \qquad (29)$$

$$\Psi_1\left(s_{in,j_h},u,p\right)\le W^L\Gamma_1\left(s_{in,j_h},u,p\right)+T^UW(u)-W^LT^U \qquad (30)$$

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.

The final completely linearised form of Constraint (7) can be seen in Constraint (31).

$$Q\left(s_{in,j_h},u,p-1\right)=c_p\left(\Psi_1\left(s_{in,j_h},u,p\right)-\Psi_2\left(s_{in,j_h},u,p-1\right)\right)\quad \forall\ p\in P, p>p0,\quad s_{in,j_h}\in S_{in,j},\quad u\in U \qquad (31)$$

The full linearisation procedure is carried out for each of the trilinear terms resulting from Constraints (6), (7) and (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 2.

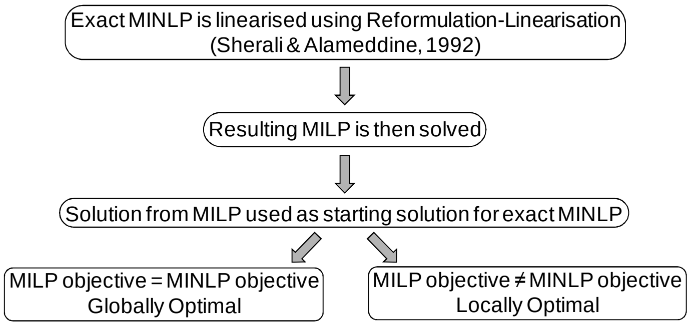

Figure 2 Solution algorithm for Reformulation-Linearisation technique

Heat Loss Considerations

Constraint (32), which is used in Constraint (10) and Constraint (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.

$$\Delta\dot{T}(u,p)=\frac{\dot{Q}_{loss}(u,p)}{W(u)c_p}\quad \forall\ p\in P, p>p0,\quad u\in U \qquad (32)$$

The idle time for the heat storage vessel, when heat is neither stored nor released, is defined by Constraint (33).

$$\Delta t(p)=t_0\left(s_{in,j},u,p\right)-t_f\left(s_{in,j},u,p-1\right)\quad \forall\ p\in P, p>p0,\quad s_{in,j_h}\in S_{in,j},\quad u\in U \qquad (33)$$

The amount of heat lost to the environment is quantified in Constraint (34).

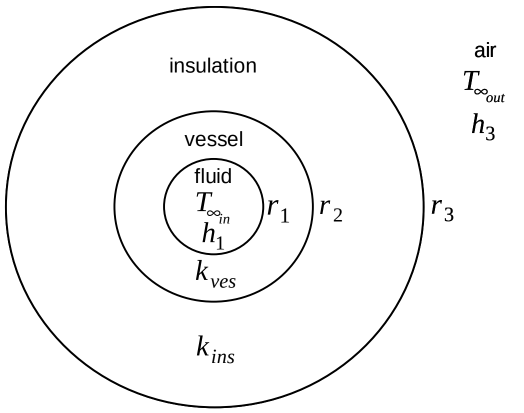

Figure 3 Insulated heat storage vessel

$$\dot{Q}_{loss}(u,p) = \frac{T_{\infty_{in}}(u,p) - T_{\infty_{out}}}{R_{tot}(u)}$$
$$\forall\ p \in P, p > p0, \quad u \in U \qquad (34)$$

$T_{\infty_{in}}$ 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 (35) with each term defined in Constraint (36).

$$R_{tot}(u) = R_{conv_1}(u) + R_{ves}(u) + R_{ins}(u) + R_{conv_3}(u)$$
$$\forall\ u \in U \qquad (35)$$

$$R_{tot}(u) = \frac{1}{h_1 A_1(u)} + \frac{\ln\left(\frac{r_2}{r_1}\right)}{2\pi L(u) k_{ves}} + \frac{\ln\left(\frac{r_3}{r_2}\right)}{2\pi L(u) k_{ins}} + \frac{1}{h_3 A_3(u)}$$
$$\forall\ u \in U \qquad (36)$$

The internal area for heat loss by convection from the heat transfer medium is given by Constraint (37) and the area for convective heat transfer losses to the environment is given in Constraint (38).

$$A_1(u) = 2\pi r_1 L(u)$$
$$\forall\ u \in U \qquad (37)$$

$$A_3(u) = 2\pi r_3 L(u)$$
$$\forall\ u \in U \qquad (38)$$

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 (39).

$$W(u) = V(u) = \pi r_1^2 L(u)$$
$$\forall\ u \in U \qquad (39)$$

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

INDUSTRIAL CASE STUDY

The flowsheet for the process is shown in Figure 4.

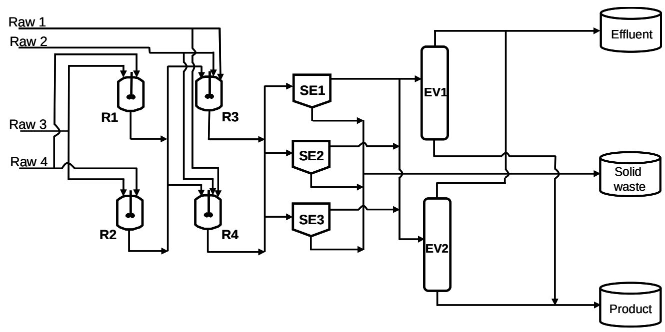

Figure 4 Flowsheet for the industrial case study

The STN for the process is shown in Figure 5 and the SSN is shown in Figure 6. The scheduling data may be obtained from Tables 1, 2 and 3 [13]. 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.

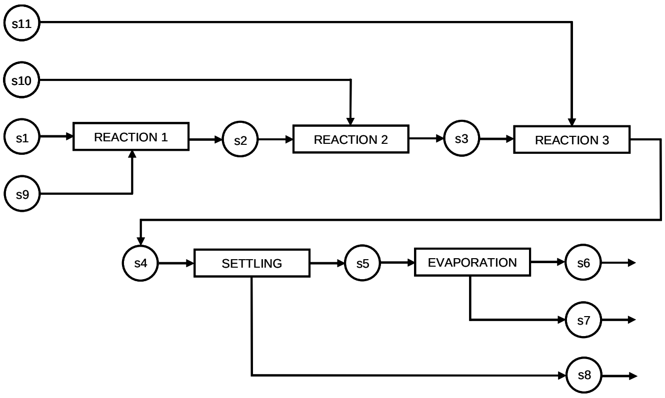

Figure 5 State task network of industrial case study

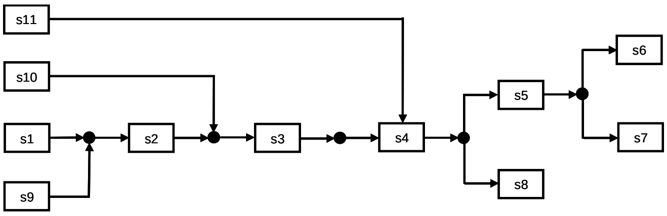

Figure 6 State sequence network of industrial case study

Table 1 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 2 Stoichiometric data for industrial case study

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

Table 3 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

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, with heating and cooling requirements summarised in Table 5.

Table 4 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 5 Heating/cooling requirements for industrial case study

Reaction	Type	Heating/Cooling Requirement (kWh)	Operating Temperature (°C)
RX2	exothermic	100 (cooling)	150
Evap.	endothermic	110 (heating)	90

Heat integration in Figure 7 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 [1]. The results for different scenarios are summarised in Table 6.

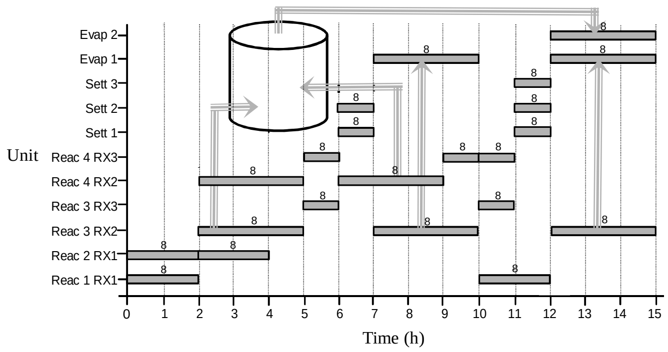

Figure 7 Schedule shows improvement in energy usage (no heat losses)

The variation in temperature of the heat storage vessel, disregarding heat losses, is shown in Figure 8.

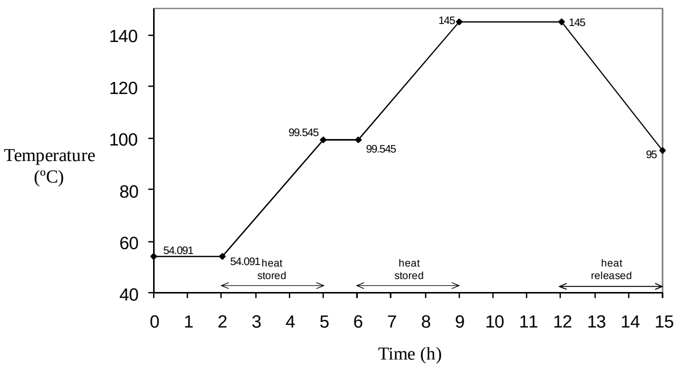

Figure 8 Temperature variation in heat storage vessel (no heat losses)

The solution procedure as described previously in Fig. 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.

Table 6 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 (ºC)			80	54.091
CPU time (s)			2805.2	95396
Binary variables				194
Time points				11

Heat Loss Considerations

Heat losses from the idle heat storage tank for the industrial case study were included with the parameters in Table 7. The time horizon of interest was decreased to 10 hours in order to reduce the solution time.

Table 7 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 8.

Table 8 Results for industrial case study with heat losses taken into account

	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 9.

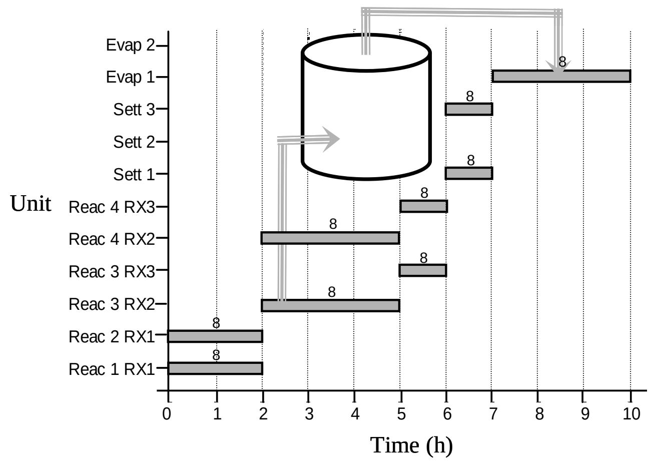

Figure 9 Optimal schedule over shorter time horizon

As can be seen from the results in Table 8, 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 10.

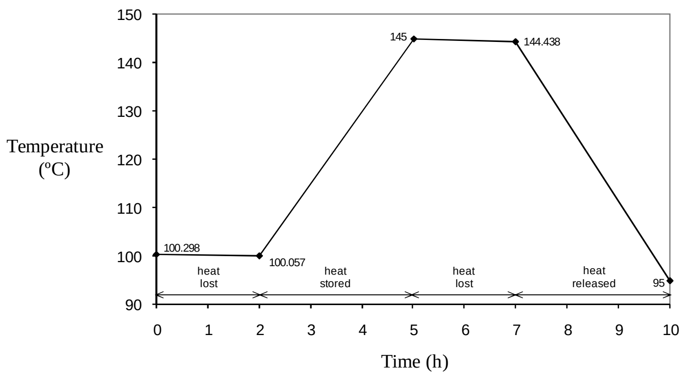

Figure 10 Temperature variation in heat storage vessel with heat losses considered

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 10, 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.

CONCLUSIONS

Most heat integration methods discussed in the literature either rely on a predefined schedule or consider either direct or indirect heat integration only, which both lead to suboptimal results. Using both direct heat integration and indirect heat integration, via heat storage, may significantly reduce utility needs in a batch processing plant [1]. 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 suboptimal parameters. The temperature drop of heat storage due to heat losses depends 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). It may be considered negligible for a well insulated vessel over short time horizons if temperatures are low.

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