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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 during idling are also considered. This work is an extension of MILP model of Majozi (2009), 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.

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1. Introduction

Chemical and process industries rank among the largest consumers of energy [2]. Most waste heat is eventually released to the atmosphere through cooling water, cooling towers, flue gases and other heat losses [3]. Batch processes are commonly used for the manufacture of products required in small quantities or for speciality or 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 [4]. 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%–10% of total costs [5–7]. 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 and heat integration has proved successful in improving energy efficiency [1,8–16]. Although the energy savings obtainable through heat integration might 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.

Many heat integration techniques lead to suboptimal results due to a predefined schedule. Various of these methods are now discussed. Early work on heat integration in batch processes [17] explored heat exchange between hot and cold vessels requiring cooling and heating, respectively, in order to reduce utility consumption. Heuristics were used when temperatures were not limiting and a MILP formulation when temperatures were limiting. Vaklieva-Bancheva et al. [7] 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 problem, 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. Only specific pairs of units were allowed to undergo heat integration. Wang and Smith [18] 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 with rescheduling were considered. Instead of analysing batch streams from a thermodynamic perspective, Uhlenbruck et al. [19] proposed first synthesising all possible heat exchanger networks using direct heat integration. The given schedule was divided into

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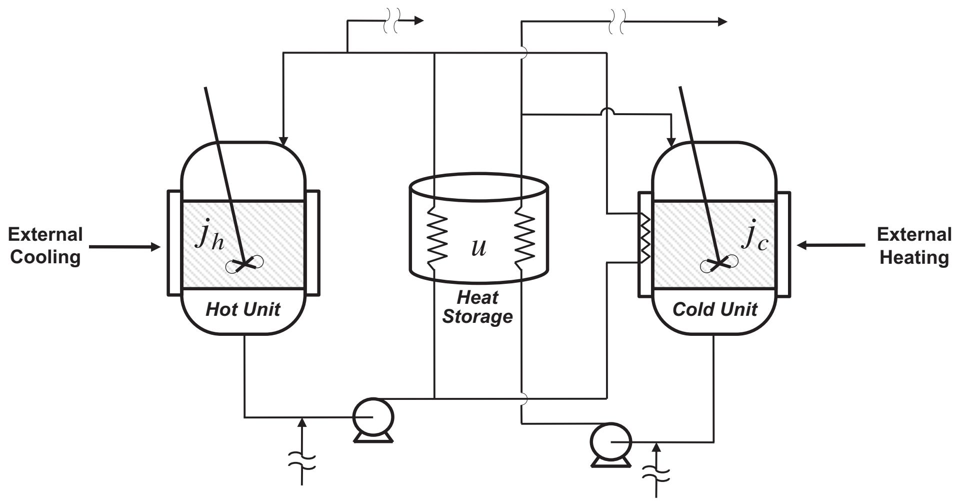

Fig. 1. Superstructure for mathematical model.

time and temperature intervals. One hot stream was allowed to exchange with one cold stream via a countercurrent heat exchanger. The heat recovery was improved further by including matches of residual and previously unmatched streams. The method could not achieve the thermodynamic optimum. De Boer et al. [3] 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 [20] 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. Halim and Srinivasan [21] discussed a sequential method using direct heat integration. A number of optimal schedules with minimum makespan were found and heat integration analysis was performed on each. The schedule with minimum utility requirement was chosen as the best. It was argued that sequential procedures could lead to a higher number of practically implementable networks with an optimal schedule and are also more suitable for complex problems.

For a more optimal solution, scheduling and heat integration may be combined into an overall problem. Papageorgiou et al. [22] embedded a heat integration model within the scheduling formulation of Kondili et al. [23]. 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

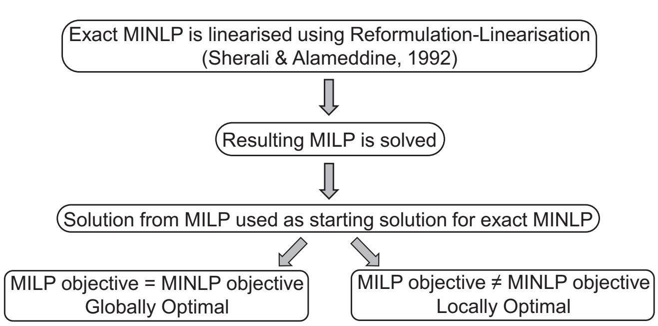

Fig. 2. Solution algorithm for Reformulation-Linearisation technique.

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 problem, 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 [24] to consider fouling of heat exchange units and the associated cleaning schedules and costs. Pinto et al. [25] 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 representation of the time horizon was used, which resulted in a large number of binary variables. Adonyi et al. [26] used the "S-Graph" scheduling approach [27] and incorporated one to one direct heat integration. Heat integration was greatly improved with a small compromise in minimal makespan. Majozi [28] presented a direct heat integration formulation based on the State Sequence Network (SSN) and an unevenly discretised time horizon [29]. The SSN scheduling formulation has been proven to require fewer binary variables compared to previous formulations based on the State Task Network (STN). The heat integration formulation as given was, however, more suited to multiproduct applications rather than multipurpose facilities. This work was later extended [1] to include heat storage for indirect heat integration. The heat storage capacity and initial storage temperature were, however, predefined parameters. Although this led to a MILP formulation, suboptimal results were obtained. Chen and Chang [30] extended the work of Majozi [28] to periodic scheduling, based on the Resource Task Network (RTN). The resultant direct heat integration formulation was a MILP problem. The SSN formulation of Majozi [28] 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.

Most of the methods discussed either rely on a predefined schedule or consider either direct or indirect heat integration only, which both lead to suboptimal results. This work is an extension of Majozi [1] to multipurpose facilities, with optimisation of the heat storage capacity available as well as the initial temperature of the heat storage medium. The problem and objectives are given in the next section. The mathematical model and linearisation techniques are then discussed. A consideration of heat losses from the heat storage vessel then follows. The model is then applied to both a literature example and an

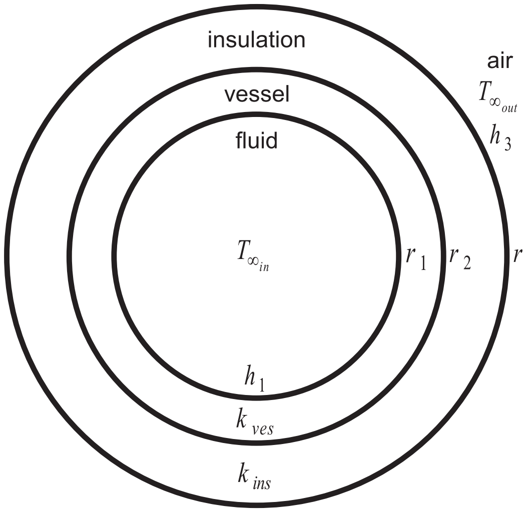

Fig. 3. Insulated heat storage vessel.

industrial case study. Conclusions are then drawn highlighting the value of the current work.

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) 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.

3. Mathematical model

The SSN recipe representation and an uneven discretisation of the time horizon were used to model the process [29]. This has proven to result in fewer binary variables compared to models based on other representations.

The model is based on the superstructure in Fig. 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.

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

3.1. Sets

$J = \{ j | j$ is a processing unit$\}$
$J_c = \{ j_c | j_c$ is a processing unit which may conduct tasks requiring heating$\} \subset J$
$J_h = \{ j_h | j_h$ is a processing unit which may conduct tasks requiring cooling$\} \subset J$
$P = \{p | p$ is a time point$\}$
$S = \{s | s$ is any state$\}$
$S_{\text{in},j} = \{s_{\text{in},j} | s_{\text{in},j}$ is an input stream to a processing unit$\} \subset S$
$U = \{u | u$ is a heat storage unit$\}$

3.2. Continuous variables

$A_1(u)$ = area for convective heat transfer from heat transfer medium
$A_3(u)$ = area for convective heat transfer to environment
$cw(s_{\text{in},j_h}, p)$ = 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
$Q(s_{\text{in},j}, u, p)$ = heat exchanged with heat storage unit u at time point p

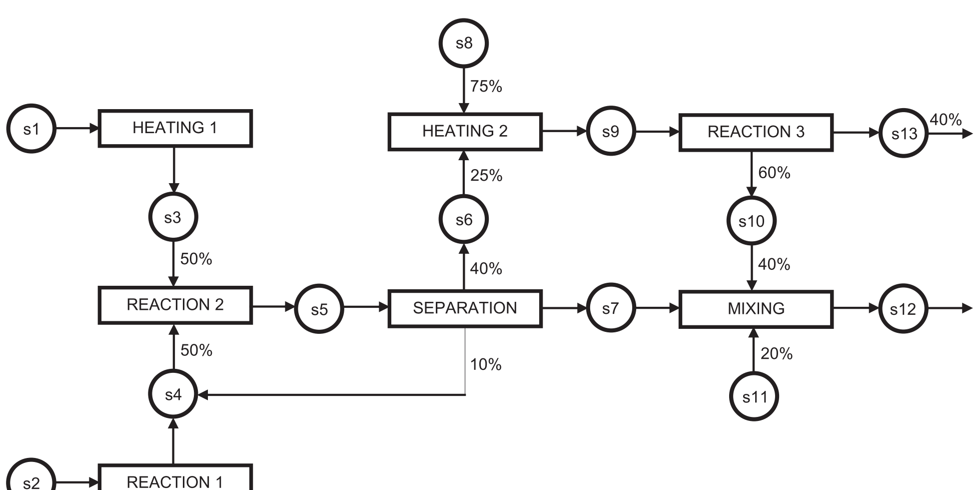

Fig. 4. State task network of multipurpose batch facility.

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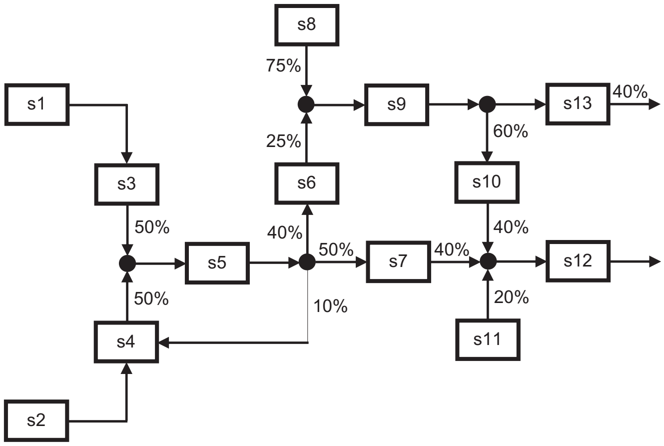

Fig. 5. State sequence network of multipurpose batch facility.

$\dot{Q}_{loss}(u,p)$ = 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

3.3. Binary variables

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

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

Table 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 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

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

3.4. 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
ΔT^{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

3.5. Constraints

In addition to the necessary short term scheduling constraints [29], Constraints (1)–(22) constitute the heat integration model,

Table 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
ΔT^{min} (°C)	10
T^L (°C)	20
T^U (°C)	180
W^L (ton)	1
W^U (ton)	3

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Table 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

Table 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

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 [28,1]. 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.

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

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

Constraint (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.

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

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

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

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

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, $z(s_{\text{in},j},u,p)$, 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.

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

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

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 $T_0(u,p0)$.

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

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.

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

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

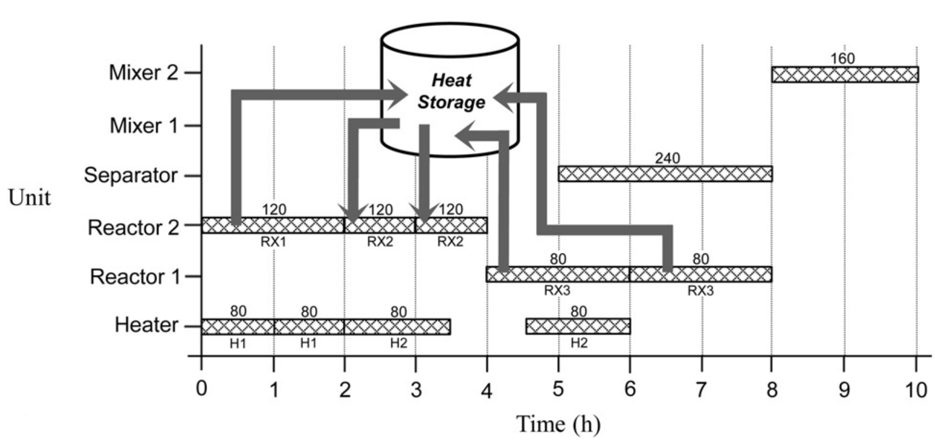

Fig. 6. Optimal schedule for literature example with heat losses.

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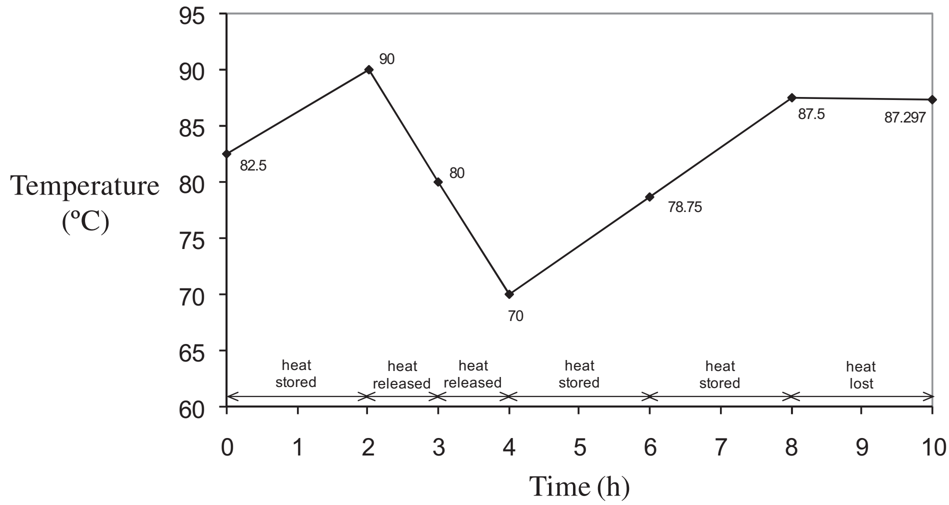

Fig. 7. Variation in heat storage vessel temperature for literature example.

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, Constraints (10) and (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.

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

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

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

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

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.

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

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

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.

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

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.

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

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.

Table 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) [a]	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

[a] Performance index = Revenue – utility costs.

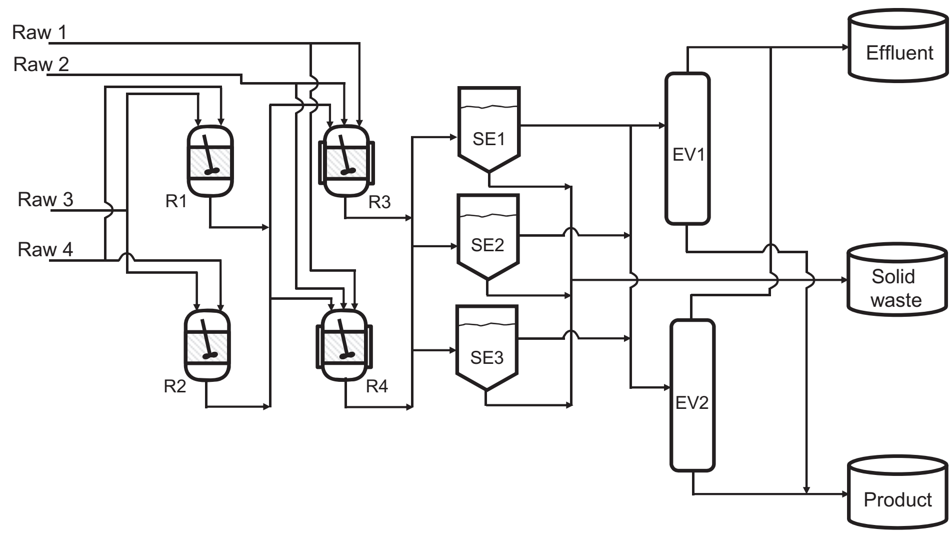

Fig. 8. Flowsheet for industrial case study.

This constraint may be relaxed for operations requiring preheating or precooling and is dependent on the process.

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

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

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.

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

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

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.

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

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

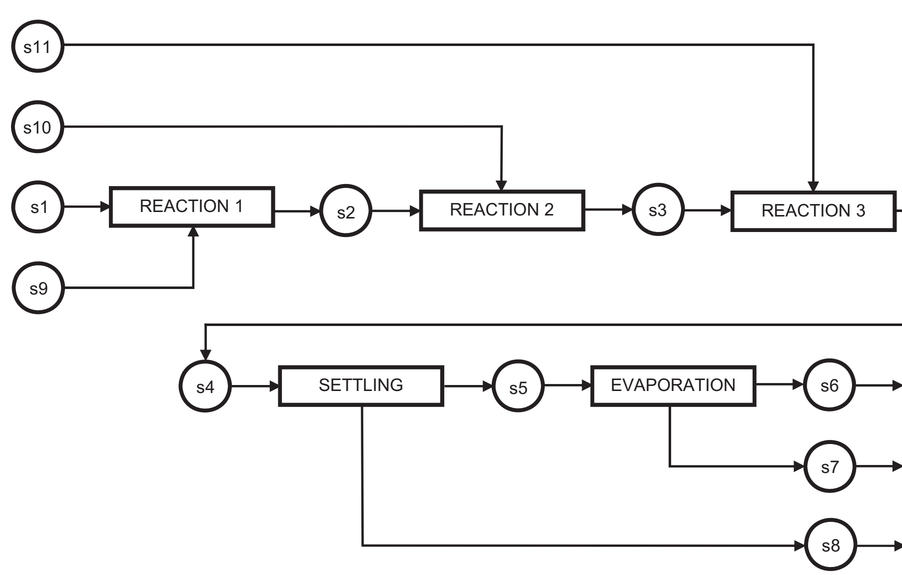

Fig. 9. State task network of industrial case study.

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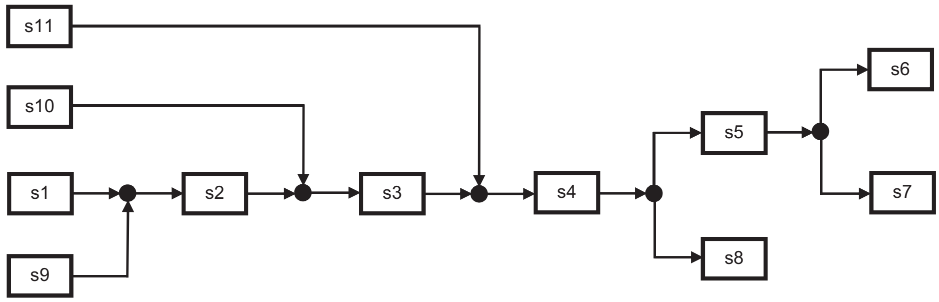

Fig. 10. State sequence network of industrial case study.

Constraints (6)–(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 [31]. This is an exact linearisation technique and as such will not compromise the accuracy of the model. The procedure is demonstrated for Constraint (7) in Appendix A, and leads to Constraint (23).

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

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 [32] as discussed by Quesada and Grossmann [33]. This is demonstrated for Constraint (23), resulting in Constraints (24)–(30).

Let

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

With lower and upper heat storage capacity and temperature bounds known

$$W^L \le W(u) \le W^U \tag{25}$$

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

Then

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

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

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

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

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).

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

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

4. Heat loss

Constraint (32), which is used in Constraints (10) and (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 Fig. 3.

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

Table 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 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

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Table 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

Table 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
ΔT^{min} (°C)	5
T^L (°C)	20
T^U (°C)	180
W^L (ton)	0.2
W^U (ton)	1

Table 11
Heating/cooling requirements for industrial case study.

Reaction	Type	Heating/Cooling requirement (kWh)	Operating temperature (°C)
RX2	Exothermic	100 (cooling)	150
Evaporation	Endothermic	110 (heating)	90

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

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

The rate of heat loss to the environment is quantified in Constraint (34).

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

$T_{\infty in}$ 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).

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

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

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).

$$A_1(u) = 2\pi r_1 L(u) \forall u \in U \tag{37}$$

$$A_3(u) = 2\pi r_3 L(u) \forall u \in U \tag{38}$$

If the density of the heat transfer fluid is assumed to be 1000 kg/m3, 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).

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

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

5. Literature example: multipurpose batch facility [34]

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 Fig. 4 and the state sequence network is shown in Fig. 5. The process requires sharing of equipment and multiple tasks and states.

Scheduling data are shown in Table 1 and Table 2 [34], while heat integration data are shown in Table 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.

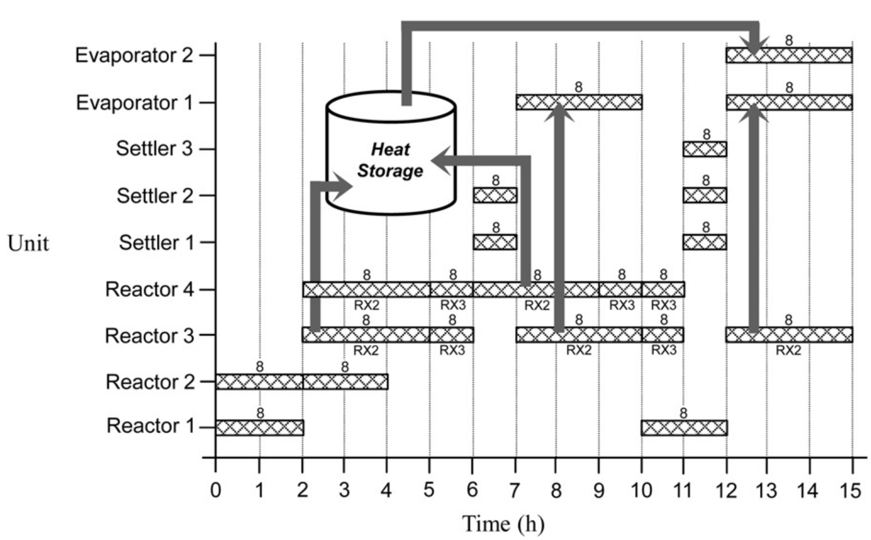

Fig. 11. Schedule shows improvement in energy usage (no heat losses).

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Table 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)[a]	131 376.471	138 176.471	139 776.471	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

[a] Performance index = Revenue − utility costs.

Parameters for heat loss considerations may be found in Table 5.

The batch sizes for all units were fixed at 80% of design capacity. The resulting optimal schedule for the literature example is shown in Fig. 6. Heat integration is indicated with arrows and one heat storage unit was used.

The variation in temperature of the heat storage vessel may be seen in Fig. 7.

The results for literature example are summarised in Table 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 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, 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.

6. Industrial case study [29]

The flowsheet for the process is shown in Fig. 8.

The STN for the process is shown in Fig. 9 and the SSN is shown in Fig. 10. The scheduling data may be obtained from Tables 7, 8 and 9 [29]. 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 2 h. The intermediate from Reaction 1 is then transferred either to Reactor 3 or Reactor 4, where two consecutive reactions take place. Reaction 2 takes 3 h and Reaction 3, 1 h. 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 1 h. This salt-free solution is then transferred to one of two Evaporators, where steam (equivalent to 110 kWh) is used to

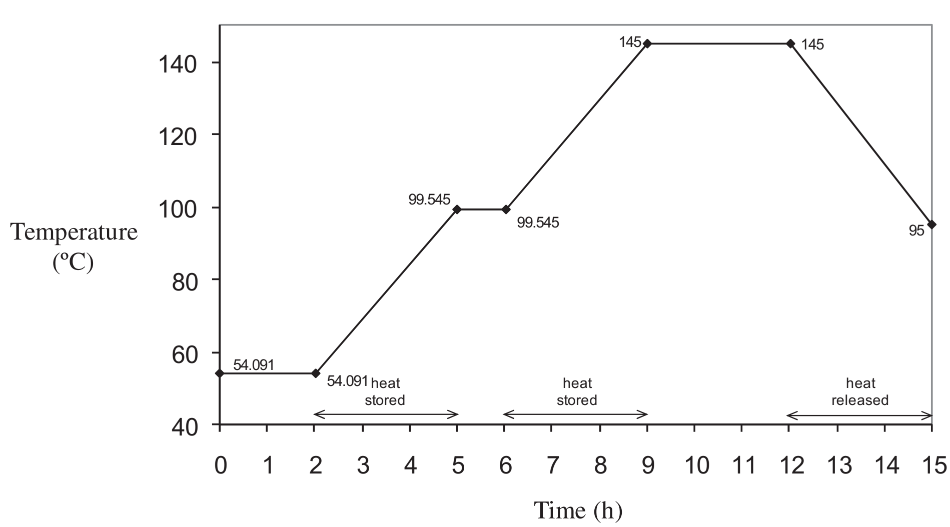

Fig. 12. Temperature variation in heat storage vessel (no heat losses).

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Table 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

Table 14
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

remove excess water from the product, which takes 3 h. 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.

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 10, with heating and cooling requirements summarised in Table 11.

Heat integration in Fig. 11 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 12.

The variation in temperature of the heat storage vessel, disregarding heat losses is shown in Fig. 12.

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.

6.1. Heat loss considerations

Heat losses from the idle heat storage tank for the industrial case study were included with the parameters in Table 13. The time horizon of interest was decreased to 10 h in order to reduce the solution time.

The results may be obtained from Table 14.

The Gantt chart for the case where heat losses from the heat storage vessel were considered can be seen in Fig. 13.

As can be seen from the results in Table 14, the shorter time horizon requires a higher starting temperature when compared to the horizon of 15 h. 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 Fig. 14.

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 Fig. 14, the temperature gradient is steeper from 5 to 7 h {(145−144.438)/2 = 0.281} when compared to 0–2 h, {(100.298−100.057)/

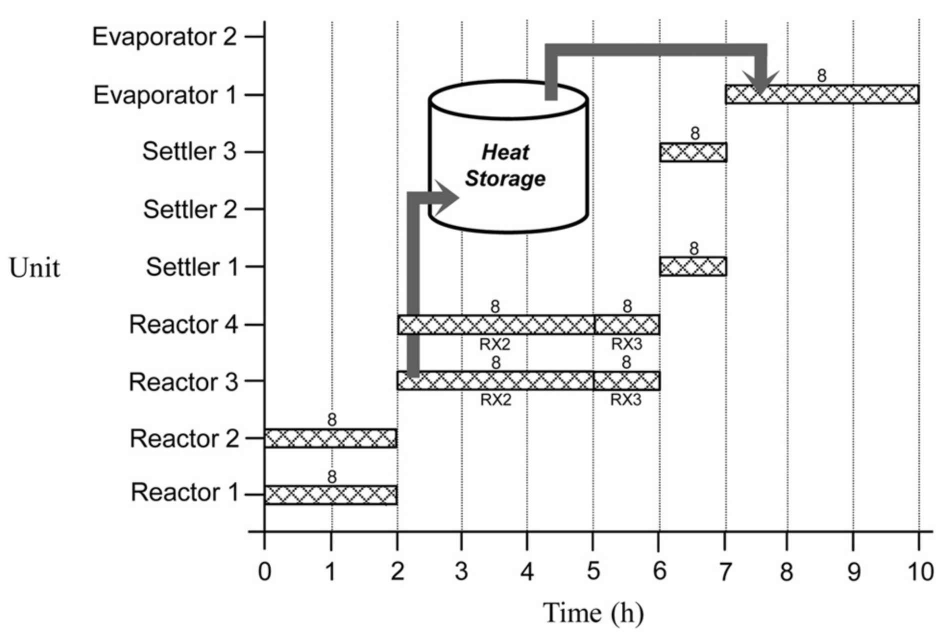

Fig. 13. Optimal schedule over shorter time horizon, with heat losses.

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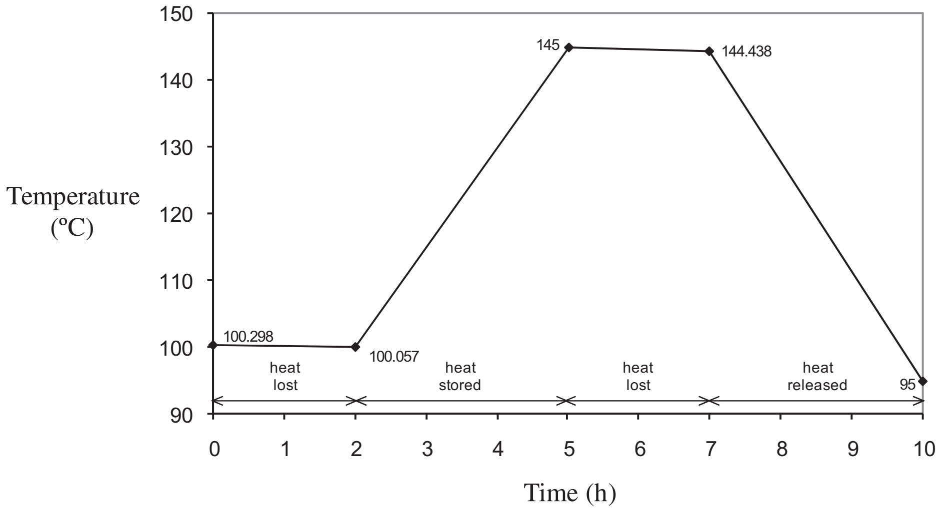

Fig. 14. Temperature variation in heat storage vessel with heat losses considered.

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 was 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.

7. 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.

Appendix A. Glover transformation [31]

From Constraint (7),
Let

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

With lower and upper temperature bounds known

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

Then

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

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

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

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

The result from the Glover transformation for Constraint (7) is seen in Constraint (A7) and includes the addition of one new continuous variable and four new continuous constraints.

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

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