Heat integration of multipurpose batch plants using a continuous-time framework

Thokozani Majozi *

University of Pretoria, Department of Chemical Engineering, Lynwood Road, Pretoria 0002, South Africa

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Abstract

Presented in this paper is a continuous-time mathematical formulation for optimization of heat integrated batch chemical plants. This formulation is applicable to both multipurpose and multiproduct facilities in which opportunities for direct heat integration exist. It is assumed that thermal driving forces and heat duties between operations identified as potential heat integration candidates are sufficient. These operations can either belong to the same batch plant or distinct batch facilities within the same site. Two scenarios are explored in this paper. The first scenario entails a situation where energy requirement is dependent on batch size, which is allowed to vary with distinct task occurrences within the time horizon of interest. The second scenario is based on fixed batch sizes in which the duty requirement is specified as a parameter. In the first scenario, the resulting formulation is initially cast as a nonconvex mixed integer nonlinear program (MINLP), which is linearized exactly to yield a convex MILP problem. This linearization is not necessary in the second scenario, as the resulting model is readily an MILP problem. A literature example and a case study are used to demonstrate the effectiveness of the formulation.

Keywords: Heat integration; Batch; Optimization; Multipurpose; Multiproduct

1. Introduction

Until recently, heat integration has always been the privilege of continuous rather than batch chemical processes. This is mainly due to the fact that, in general, heat integration techniques assume steady-state behaviour, which is a feature of continuous processes. Moreover, batch operations tend to be less energy-intensive than their continuous counterparts. However, the increasing popularity of batch plants and the continuing global emphasis on emissions reduction is starting to warrant either the adaptation of the well-established heat integration techniques to or the development of novel techniques for batch processes. The increase in popularity is due to the flexibility and adaptability of batch plants, which is crucial in the current volatile market trends. It is also worthy of note that, although external utility requirement is a secondary economic issue in most batch facilities, e.g. agrochemicals and pharmaceuticals, it can be significant in others, e.g. dairy and brewing [11].

Early work on heat integration of batch plants was proposed by Vaselanak et al. [18]. These authors explored heat integration of batch vessels containing hot fluid that required cooling and cold fluid that required heating. Four cases were investigated. In the first case, the fluid from one vessel was allowed to return to the same vessel after exchanging heat with the fluid of another vessel via a common heat exchanger. In the second case, a heating or cooling medium was used to transfer heat between the hot fluid vessel and the cold fluid vessel, thereby maintaining the heat integrated fluids within...
the vessels throughout the heat exchange process. The third case entailed the transfer of fluids from their original vessels to receiving vessels while being heated or cooled. The fourth case was the combination of the above cases. Implicit in their analysis was the given schedule of the operations. A heuristic procedure was proposed for the cases where the final temperatures were not limiting and an MILP formulation for the cases where the final temperatures were limiting. Subsequent to this, other mathematical formulations for heat integration of batch processes have been proposed by Peneva et al. [14], Ivanov et al. [3], Corominas et al. [2], Papageorgiou et al. [13], Vaklieva-Bancheva et al. [17], Barbosa-Póvoa et al. (2001) and Adonyi et al. [1].

Peneva et al. [14] and Ivanov et al. [3] addressed the problem of designing a minimum total cost heat exchanger network for given pair wise matches of batch vessels. An implicit predefined schedule was also assumed. Corominas et al. [2] considered the problem of designing a minimum cost heat exchanger network and a heat exchange strategy for multiproduct batch plants operating in a campaign mode. The objective was to maximize heat exchange in a pre-specified campaign of product batches with hot streams requiring cooling and cold streams requiring heating. The emphasis on campaign mode implies that the proposed methodology cannot be applied in situations where equipment scheduling is of essence. Papageorgiou et al. [13] extended the discrete-time formulation of Kondili et al. [7] for scheduling of multipurpose batch plants by including heat integration aspects. Direct and indirect heat integration configurations were addressed. The main drawback of all discrete-time formulations is their explosive binary dimension, which requires enormous computational effort. Vaklieva-Bancheva et al. [17] improved the work of Ivanov et al. [3] by embedding the heat integration framework within an overall scheduling framework. However, the authors only addressed a special case in which the plant is assumed to operate in a zero-wait overlapping mode, where each product must pass through a subset of the equipment stages, and production is organized in a series of long campaigns. Recently, Pinto et al. [15] presented a discrete-time mixed integer mathematical formulation for the design of heat integrated multipurpose plants based on superstructure approach. A graph theory based technique that
incorporates heat integration within scheduling of multipurpose plants has also been proposed by Adonyi et al. [1] with emphasis on make span minimization.

Other established attempts on heat integration of batch plants are based on the concept of pinch analysis [8], which was initially developed for continuous processes at steady-state. As such, these methods assume a pseudo-continuous behaviour in batch operations either by averaging time over a fixed time horizon of interest [9] or assuming fixed production schedule within which opportunities for heat integration are explored [5,6,12,4]. It is, therefore, evident that these methods cannot be applied in situations where a production schedule that maximizes heat integration whilst optimizing production demands is sought.

The methodology presented in this paper is based on a continuous-time scheduling framework developed by Majozi and Zhu [10] and is applicable to both multi-product and multipurpose batch processes. Two cases are considered. The first case entails a situation where energy requirement is dependent on batch size, which is allowed to vary with distinct task occurrences within the time horizon of interest. The second case is based on fixed batch sizes in which the duty requirement is specified as a parameter. In the first case, the mathematical model is initially cast as a mixed integer nonlinear program (MINLP) and then linearized exactly to yield a mixed integer linear program (MILP) to guarantee global optimality. In the second case, the mathematical model is readily an MILP. The developed model has three major advantages compared to other methodologies published in literature. Firstly, it is based on a continuous-time framework, which results in much fewer binary variables than the discrete-time formulation, hence the reduced computational effort. Secondly, it is not strictly constrained on time, i.e. the time horizon can be increased and reduced as necessitated by the problem at hand. This feature allows the model to capture the cyclic state behaviour, which is inherent in batch processes. Thirdly, the objective function can assume several forms depending on the nature of the application, e.g. minimization of make span, maximization of profit, minimization of capital cost investment, etc. A case study to demonstrate the capability of the developed model is also presented.

2. Problem statement

The problem addressed in this paper can be stated as follows. Given:

(i) production scheduling data, i.e. equipment capacities, task durations, time horizon of interest, recipe for each product as well as cost of raw materials and selling price of final products,
(ii) hot and cold duties for tasks that require heating and cooling, respectively and
(iii) cost of cooling water and steam,

determine the production schedule that is concomitant with maximum process–process heat transfer and maximum profit. In the context of this paper, profit is defined as the difference between revenue and operating costs. The latter constitute raw material costs and external utility (cooling water and steam) costs. It is assumed that sufficient temperature driving forces exist between matched tasks for process–process heat transfer. Also, each task is allowed to operate either in an integrated or standalone mode. If heat integration cannot supply sufficient duty, external utility is supplied to complement the deficit. Whilst heat integrated tasks have to be active within a common time interval to effect direct heat transfer, they need not necessarily commence nor end at the same time. Moreover, the heat integrated tasks can either belong to the same process or distinct processes within reasonable proximity.

3. Mathematical formulation

The presented mathematical formulation is an extension of the scheduling model proposed by Majozi and Zhu [10], which uses a state sequence network (SSN) representation. This formulation is based on a continuous-time framework [16] as shown in Fig. 1. A time point corresponds to the beginning of a particular task and is not necessarily equidistant from the preceding and the succeeding time points, as it encountered in discrete-time formulations. The details of the scheduling formulation without heat integration will not be presented in this paper as they appear elsewhere [10]. Two cases are considered. The first case involves a situation where the batch size is allowed to vary at different
instances along the time horizon of interest. The second case is based on fixed batch sizes.

3.1. Case 1: variable batch size

\[ \sum_{j \in J_h} x(j, f', p) \leq y(s_{m,j}, p), \quad \forall p \in P, \ j \in J_h, \ s_{m,j} \in S_{m,j} \]

(1)

\[ \sum_{j \in J_c} x(j, f', p) \leq y(s_{m,j}, p), \quad \forall p \in P, \ j \in J_c, \ s_{m,j} \in S_{m,j} \]

(2)

Constraint (1) states that if unit \( j \), which requires heating, is integrated with any unit \( j' \) requiring cooling at time point \( p \), then unit \( j \) must be active at that time point. However, the fact that unit \( j \) is active at time point \( p \) does not necessarily mean that it operates in an integrated mode, as standalone operation is allowed. Constraint (2) is similar to constraint (1), but applies to unit \( j' \). It is also worthy of note that the above constraints ensure a one-to-one heat integration arrangement between heat integrated units. This is indeed a preferred option for plant operability purposes.

\[ q(j, p) = K_{1,j} \left( y(s_{m,j}, p) - \sum_{j' \in J_h} x(j', f', p) \right) \]

+ \( K_{2,j} \sum_{s_{m,j}} m_u(s_{m,j}, p) \left( y(s_{m,j}, p) - \sum_{j' \in J_h} x(j', f', p) \right), \quad \forall p \in P, \ j \in J_h, \ s_{m,j} \in S_{m,j} \]

(3)

\[ q'(j, p) = K_{1,j}^' \sum_{j' \in J_h} x(j', f', p) \]

+ \( K_{2,j}^' \sum_{s_{m,j}} m_u(s_{m,j}, p) \sum_{j' \in J_h} x(j', f', p), \quad \forall p \in P, \ j \in J_h, \ s_{m,j} \in S_{m,j} \]

(4)

Constraints (3) and (4) are expressions of the external utility requirement for unit \( j \), which requires heating, when operating in a standalone and integrated mode, respectively.

\[ q(j', p) = K_{1,j'} \left( y(s_{m,j'}, p) - \sum_{j' \in J_h} x(j, f', p) \right) \]

+ \( K_{2,j'} \sum_{s_{m,j'}} m_u(s_{m,j'}, p) \left( y(s_{m,j'}, p) - \sum_{j' \in J_h} x(j, f', p) \right), \quad \forall p \in P, \ j \in J_h, \ s_{m,j} \in S_{m,j} \]

(5)

\[ q'(j', p) = K_{1,j'}^' \sum_{j \in J_h} x(j, f', p) \]

+ \( K_{2,j'}^' \sum_{s_{m,j'}} m_u(s_{m,j'}, p) \sum_{j \in J_h} x(j, f', p), \quad \forall p \in P, \ j \in J_h, \ s_{m,j} \in S_{m,j} \]

(6)

Constraints (5) and (6) are similar to constraints (3) and (4), but apply to unit \( j' \), which requires cooling, when operating in a standalone and integrated mode, respectively. It is evident that constraints (3)–(6) involve bilinear terms comprising a continuous and a binary variable. These terms can be exactly linearized using Glover transformation to yield an overall model for which global optimality can be guaranteed as shown below.

3.1.1. Linearization using Glover transformation

The bilinear terms in constraints (3) and (4) are replaced by variables \( \Gamma_1 \) and \( \Gamma_2 \) as shown in constraints (7) and (8). These variables are the linearly defined in constraints (11)–(14). Variables \( \Gamma_3 \) and \( \Gamma_4 \) replacing the bilinear terms in constraints (5) and (6) are introduced in constraints (9) and (10). The linear definitions of these variables are similar to those for \( \Gamma_1 \) and \( \Gamma_2 \).

\[ q(j, p) = K_{1,j} \left( y(s_{m,j}, p) - \sum_{j' \in J_h} x(j', f', p) \right) \]

+ \( K_{2,j} (\Gamma_1(s_{m,j}, p) - \Gamma_2(j, f', p)), \quad \forall p \in P, \ j \in J_h, \ s_{m,j} \in S_{m,j} \]

(7)

\[ q'(j, p) = K_{1,j}^' \left( \sum_{j' \in J_h} x(j', f', p) \right) + K_{2,j}^' \Gamma_2(j, f', p), \quad \forall p \in P, \ j \in J_h, \ s_{m,j} \in S_{m,j} \]

(8)

\[ q(j', p) = K_{1,j'} \left( y(s_{m,j'}, p) - \sum_{j' \in J_h} x(j, f', p) \right) \]

+ \( K_{2,j'} (\Gamma_3(s_{m,j'}, p) - \Gamma_4(j, f', p)), \quad \forall p \in P, \ j \in J_h, \ s_{m,j} \in S_{m,j} \]

(9)

\[ q'(j', p) = K_{1,j'}^' \sum_{j \in J_h} x(j, f', p) + K_{2,j'}^' \Gamma_4(j, f', p), \quad \forall p \in P, \ j \in J_h, \ s_{m,j} \in S_{m,j} \]

(10)

Constraints (7) and (8) are an overall model for which global optimality can be guaranteed as shown below.
0 ≤ \( \Gamma_2(s_{in,j}, p) \) ≤ \( V_j^{max} \sum_{j' \in J_c} x(j', j, p) \),
\[ \forall p \in P, \ j \in J_h, \ s_{in,j} \in S_{in,j} \] (14)

Constraints (1), (2), (8)-(14), in conjunction with the overall plant scheduling constraints, constitute a complete MILP formulation for direct heat integration in batch processes in a situation where the batch size is allowed to vary at different instances along the time horizon of interest.

3.2. Case 2: fixed batch size

In a situation where the batch size processed in a particular unit at various time points along the time horizon is fixed, the heat duty requirement will also be fixed. Therefore, it is specified as a parameter rather than a variable. Constraints (1) and (2) still hold in this scenario. However, the following additional constraints are also necessary:

\[ Q_{hi}(j) x(j, j', p) = q(j, p) + \sum_{j' \in J_c} q_{hi}(j, j', p), \]
\[ \forall p \in P, \ j \in J_h, \ s_{in,j} \in S_{in,j} \] (15)

\[ Q_{hi}(j) x(j, j', p) = q(j, p) + \sum_{j' \in J_c} q_{hi}(j, j', p), \]
\[ \forall p \in P, \ j \in J_h, \ s_{in,j} \in S_{in,j} \] (16)

\[ Q_{hi}^{min}(j, j') x(j, j', p) \leq q_{hi}(j, j', p) \leq Q_{hi}^{max}(j, j') x(j, j', p), \]
\[ \forall p \in P, \ j \in J_h, \ j' \in J_c \] (17)

Constraint (15) states that the amount of cold duty required by unit \( j' \) at any point along the time horizon of interest is comprised of external cold utility and cold duty from heat integration with another unit \( j \). Constraint (16) is similar to constraint (15) and applies to unit \( j \) requiring heating. Constraint (17) is a feasibility constraint, which ensures that in the absence of heat integration all the heat duty requirements of either unit \( j \) or \( j' \) are satisfied by external utilities. The upper bound on the amount of heat exchanged between unit \( j \) and unit \( j' \) will always be the minimum of the required cold and hot utilities as captured in Eq. (17').

\[ Q_{hi}^{max}(j, j') = \min_{j' \in J_c} \{ Q_{hi}(j'), Q_{hi}(j) \} \] (17')

The lower bound, on the other hand, is at the discretion of the designer. Constraints (1), (2) and (15)-(17'), in conjunction with the overall plant scheduling constraints, constitute a complete MILP formulation for direct heat integration in batch processes in a situation where the batch size is fixed along the time horizon of interest.

In order to ensure that the heat-integrated units are active within a common time interval, the following constraint is necessary. In constraint (18), unit \( j \) has a relatively longer duration time than unit \( j' \). If duration times are equal, then constraints (19) and (20) are necessary.

\[ t_p(s_{out,j}, p) \geq t_p(s_{out,j}, p) - H(1 - x(j, j', p)), \]
\[ \forall p \in P, \ j \in J_h, \ j' \in J_c \] (18)

\[ t_p(s_{out,j}, p) \geq t_p(s_{out,j}, p) - H(1 - x(j, j', p)), \]
\[ \forall p \in P, \ j \in J_h, \ j' \in J_c \] (19)

\[ t_p(s_{out,j}, p) \leq t_p(s_{out,j}, p) + H(1 - x(j, j', p)), \]
\[ \forall p \in P, \ j \in J_h, \ j' \in J_c \] (20)

In a situation where duration time varies with the mode of operation, the duration constraint has to be modified as shown in constraints (21) and (22) for units \( j \) and \( j' \), respectively.

\[ t_p(s_{out,j}, p) = t_u(s_{in,j}, p) \]
\[ + \tau(s_{in,j}) \left( y(s_{in,j}, p) - \sum_{j' \in J_c} x(j, j', p) \right) \]
\[ + \tau'(s_{in,j}) \sum_{j' \in J_c} x(j, j', p), \]
\[ \forall p \in P, \ j \in J_h, \ s_{in,j} \in S_{in,j}, \ s_{out,j} \in S_{out,j} \] (21)

\[ t_p(s_{out,j}, p) = t_u(s_{in,j}, p) \]
\[ + \tau(s_{in,j}) \left( y(s_{in,j}, p) - \sum_{j' \in J_c} x(j, j', p) \right) \]
\[ + \tau'(s_{in,j}) \sum_{j' \in J_c} x(j, j', p), \]
\[ \forall p \in P, \ j' \in J_c, \ s_{in,j} \in S_{in,j}, \ s_{out,j} \in S_{out,j} \] (22)

The performance of the presented formulation was tested by applying it to a literature example and an industrial case study. All solutions were obtained using the GAMS/CPLEX solver in a 1.4 GHz Pentium M processor.

4. Literature example

The following example has been extracted directly from literature [13] and is presented to demonstrate the effectiveness of the proposed formulation. It entails a plant manufacturing two products, Product1 and Product2, according to the following recipe which corresponds to the STN and SSN [10] shown in Fig. 2. The recipe as well as heat requirements are shown in Table 1. The minimum allowable size of batches processed in the reactor and the column cannot be less than 25% of their normal capacity. The corresponding figure for the filter is 10%. Sufficient dedicated storage is provided
for all raw materials and final products, while storage vessels of 100 t are available for each of the two intermediates. Unlimited availability of steam and cooling water is assumed, with corresponding unit costs of 200 and 4 relative cost units (rcu) per metric ton, respectively. The time horizon of interest is 48 h. The unit values for the two products are assumed to be equal at 5 rcu/t. An opportunity of exchanging heat exists between the Reaction task which requires cooling, and the Distillation task, which requires heating, assuming appropriate temperature levels. An equipment configuration that would permit this heat exchange to be realized is illustrated in Fig. 3.

The objective function for the literature example is the maximization of profit, which is defined as the difference between revenue and operating cost. The operating cost consists of consumed external utility costs.

4.1. Results and discussion

The literature example results for the scenario without heat integration are summarized in Table 2. The discrete-time model proposed by Papageorgiou et al. [13] involved 142 binary variables and its solution was based on a 5% margin of optimality in the branch and bound procedure. An integrality gap of 4.76% was observed.

More significantly, a suboptimal objective value of 2944.1 rcu was reported as an optimal solution. Using the continuous-time formulation proposed in this paper, a globally optimal value of 3081.8 rcu was obtained in 24.5 CPU s. Only 72 binary variables were necessary and the model solution was based on 0% margin of optimality. An integrality gap of 0% was observed. The Gantt chart corresponding to the globally optimal solution is shown in Fig. 4.

Table 3 shows the results obtained for the scenario involving heat integration. Both the discrete-time formulation proposed by Papageorgiou et al. [13] and the continuous-time formulation presented in this paper gave an objective value of 3644.6 rcu, which is an improvement of 18.3% from the standalone scenario. However, the continuous-time formulation only involves 96 instead of 188 binary variables. As a result the solution of this model was based on 1.3% instead of 5% margin of optimality. A 0% integrality gap was observed. The Gantt chart for the heat-integrated sche-
The Reaction task batches that operate in a standalone mode are marked with an X, whilst the rest operate in a heat-integrated mode. All the Distillation task batches operate in a heat-integrated mode. It is evident from the Gantt chart that the aforementioned condition of common time intervals is obeyed in all the instances that involve heat integration.

5. Industrial case study

Fig. 6 is the flowsheet for the industrial case study used to illustrate the application of the method proposed. Fig. 7 is the corresponding SSN. Table 4 shows the scheduling data. An opportunity for heat integration exists between Reaction2 task, which is conducted in R3 and R4 units, and Evaporation task, which is conducted...
in EV1 and EV2 units. The cooling load required in Reaction2 task is 5 energy units, whilst the heating load required for the Evaporation task is 4 energy units. Cooling water and steam are used for cooling and heating and cost 15 and 8 rcu, respectively. Product (state s6) selling price is 100 rcu. The time horizon of interest is 15 h. The capacity of each batch processed in the processing units is 80% of the 10 t design capacity.

5.1. Results and discussion

The case study was solved using the continuous-time formulation presented in this paper. The mathematical model for the scenario without heat integration (stand-alone mode) involved 88 binary variables and gave an objective value of 1060 rcu. This value corresponds to the production of 14 t of product and external utility consumption of 12 energy units of steam and 20 energy units of cooling water. On the other hand, the model for the heat-integrated scenario required 120 binary variables and gave an objective value of 1256 rcu, which corresponds to 18.5% improvement in objective value. The product throughput was unaltered, but the external utility consumption was reduced to 0 t for steam and 18 t for cooling water. The absolute elimination of steam requirement is due to the fact that all Evaporation task batches operate in a heat-integrated mode. A 0% margin of optimality in the branch and bound procedure was used and a 0% integrality gap observed in both the heat-integrated and standalone scenarios. The results were obtained within 26 CPU s.

The Gantt chart for the heat-integrated schedule is shown in Fig. 8. All the Evaporation tasks are conducted in a heat-integrated mode. The first batch of the Evaporation task in EV2 exchanges heat with the third batch of Reaction2 task in R3, whilst the second batch in EV2 exchanges heat with the third batch of Reaction2 task in R4. Only one batch of the Evaporation task is processed in EV1. This batch exchanges heat with the last batch of the Reaction2 task in R3.
6. Conclusions

A continuous-time mathematical formulation for direct heat integration of multipurpose batch plants has been presented. The formulation results in smaller problems compared to the discrete-time formulation, which renders it applicable to large-scale problems. Application of the formulation to an industrial case study showed an 18.5% improvement in objective function for the heat-integrated scenario relative to the standalone scenario.

References