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Simultaneous Heat Integration and Batch Process Scheduling

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Heat integration of continuous processes is a widely studied research area, where many approaches have been developed to minimize cold and hot utility usage. Batch processes require additional consideration for the planning of the heat exchanger network: since the flows are not always present in the system, their timing has to be considered as well.

Both heat integration and scheduling of batch processes are highly complex, their combination is expected to be even higher. Several papers have already addressed the integrated problem in the last decade (Majozi, 2006, Chen and Chang, 2009, Halim and Srinivasan, 2011). Adonyi et. al. (2003) has presented an algorithm to minimize the utility usage for a given time horizon. Their approach assumed, however, that heat exchangers are present for all of the hot-cold stream pairs. Moreover, each hot or cold stream was allowed to be matched with only one hot or cold stream, respectively, further heat demands of the stream had to be satisfied from utilities.

The aim of this work is to present an extension of Adonyi *et. al.*'s approach by allowing the streams to have heat exchanges with multiple other streams. The newly presented approach also takes into account the limitation on the number of available heat exchangers and their scheduling.

1. Introduction

Heating and cooling are among the most significant energy demands of a chemical plant. Linhoff made an enormous contribution to reduce the energy requirements of a chemical process by introducing and developing the Pinch technology for the synthesis of Heat Exchanger Networks (HENS) starting in the 80's of the 20th century. Although, HENS gained the focus of the chemical engineering literature, and many approaches has been published to tackle this type of problems (see e.g., Smith (2005), Klemeš *et. al.* (2010)), the problem is still far from being solved, especially in the case of batch processes.

Batch processes pose an additional difficulty for heat integration, since the system is not steady state, i.e., the flows are present only for a short period of time not the whole time horizon. As a result, the scheduling decisions and heat integration need to be carried out simultaneously to achieve the energy optimal operation of the system. Some of the published approaches rely on a decomposed method, where a schedule is identified a-priori to heat integration. Although these approaches can adapt techniques developed for continuous processes, the optimality cannot be guaranteed.

Another class of papers present MILP or MINLP based formulations for the simultaneous scheduling and heat integration of batch plants, see e.g., Chen and Chang (2009), Georgiadis and Papageorgiou (2001), Halim and Srinivasan (2011), Majozi (2006), Peneva et. al. (1992). These approaches differ in addressing the heat integration, e.g., considering one-to-one heat exchanges of streams, applying heat storage vessels.

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Present work minimizes the utility usage for a given time horizon and the number of batches to be produced for each product. Note, that the feasibility of the problem requires the time horizon to be at least the minimal makespan, which is usually achieved by using only utilities to satisfy the heat demands. A cold or hot stream may exchange heat with another hot or cold stream, if they are present at the same time, and they can be assigned to one of the heat exchangers. Unlike in the previous approach by Adonyi et. al. (2003), present approach simultaneously considers the scheduling of heat exchangers and the processing units. If it is not practically prohibited, the algorithm can consider one-to-many heat exchanges as well.

2. Problem definition

The goal is to minimize the hot and cold utility usage for a given production within a given time horizon. The scheduling problem is given by a master recipe containing the set of products, intermediate- and raw materials, tasks, and processing units. Further necessary parameters as batch numbers, batch sizes, processing-, transfer-, and cleaning times are also given.

A process material needs heating or cooling, when its temperature is required to be different for being the input of the upcoming task. For this type of tasks the initial- and target temperatures, and their specific heats are given. It is assumed, that two streams can exchange heat only if the difference between their source- and target temperatures is at least ΔT_{min}. Heat exchanges take place in one of the available heat exchangers. Physical and chemical properties of the process materials may set further limitations on the pairs of streams can go through the same heat exchanger. If there is a heat exchange between two materials, the exchanged heat is proportional to the time of the heat exchange. Batch sizes and transfer times are fixed, thus the heat transfer coefficient can be calculated based on the temperature and flowrate data. Due to operational considerations, a material can flow through only at most one heat exchanger. However, it may exchanges heat with several other streams. If the exchanged heat is not sufficient, high pressure gas or cooling water can be utilized to fulfil the temperature demands of the upcoming task.

3. Proposed approach

The proposed approach relies on both the S-graph framework and linear programming tools. The problem is formulated as a MILP model, however, it is not directly given to the MILP optimization tools. The discrete decisions are carried out by an S-graph based Branch-and-Bound algorithm, and the bounds of the binary variables of the master MILP model are updated accordingly for each subproblem. The relaxation of these MILP models are used to provide bounds at the internal nodes of the tree, and the value of a solution at the leafs.

3.1 MILP master problem

The basis of the MILP master problem is a so-called general precedence based formulation, where binary variables are assigned to the allocation and sequencing of tasks; and continuous variables represent the starting and finishing time of a task or a material transfer. This part of the mathematical model is omitted here, similar models can be found in Mendez and Cerda (2003), Kopanos and Puigjaner (2010). The basic formulation is extended by continuous variables TTS_s and TTF_s to represent the starting and finishing of a transfer of material *s,* respectively.

In the heat integration part of the model, indices *c* and *h* denote cold and hot streams, and *n* is represents one of the available heat exchangers.

Binary variable $A_{h,c,n,}$ denotes the assignment of heat exchanger *n* to the hot-cold stream pair *h,c*. A heat exchanger can be used for compatible stream pairs, e.g., the streams of the same materials of different batches of the same products, thus, a binary variable is needed for the sequencing of these exchanges. Variable $P_{h,c,n,h',c'}$, takes the value of 1, if the heat exchange between *h,c* takes place earlier in *n* then the exchange between *h',c'*. Continuous variables $THS_{h,c,}$ *and* $THF_{h,c,}$ represent the starting and finishing time of heat exchange between streams *h,c*, respectively. The amount of exchanged heat is denoted by $Q_{h,c}$, that is naturally proportional to the heat transfer coefficient $d_{h,c}$ between the streams, and the shared time of the streams in the heat exchanger:

$$Q_{h,c} = d_{h,c} \cdot \left(THF_{h,c} - THS_{h,c}\right) \tag{1}$$

The starting and finishing time of the heat exchange is bounded by the starting and finishing time of the transfers of materials *h* and *c*, as it is described in Eqs. 2-5 (*H* is a parameter for the time horizon).

$$THS_{h,c} \geq TTS_c - H \cdot \left(1 - \sum_{n \in N} A_{h,c,n}\right) \tag{2}$$

$$THS_{h,c} \geq TTS_h - H \cdot \left(1 - \sum_{n \in N} A_{h,c,n}\right) \tag{3}$$

$$THF_{h,c} \leq TFS_c + H \cdot \left(1 - \sum_{n \in N} A_{h,c,n}\right) \tag{4}$$

$$THF_{h,c} \leq TFS_h + H \cdot \left(1 - \sum_{n \in N} A_{h,c,n}\right) \tag{5}$$

If two streams does not meet in any heat exchangers, the corresponding $THS_{h,s}$ and $THF_{h,c}$ variables are set to 0 by Eq. 6.

$$THF_{h,c} + THS_{h,c} \leq 2 \cdot H \cdot \sum_{n \in N} A_{h,c,n} \tag{6}$$

After the possible heat exchanges, the rest of the heat demand is fulfilled by utilities. The time spent on using hot and cold utilities to cool down or heat up streams is denoted by TU_s. The heat balance equation for stream *s* is given in Eqs. 7 and 8.

$$q_c = \sum_{h \in S_c^h} Q_{h,c} + d_h \cdot TU_c \tag{7}$$

$$q_h = \sum_{c \in S_h^c} Q_{h,c} + d_c \cdot TU_h \tag{8}$$

Where parameter q_s is the heat demand of a stream *s*, and d_c, d_h are the heat transfer coefficients with the cold and hot utilities, respectively.

The objective is to minimize the overall utility usage:

$$\sum_{c \in S^c} d_h \cdot TU_c + \sum_{h \in S^h} d_c \cdot TU_h \cdot$$

3.2 S-graph based branching

The Branch-and-Bound procedure is driven by an S-graph based branching algorithm. The approach is based on an extended S-graph representation of a process, shown in Figure 1.

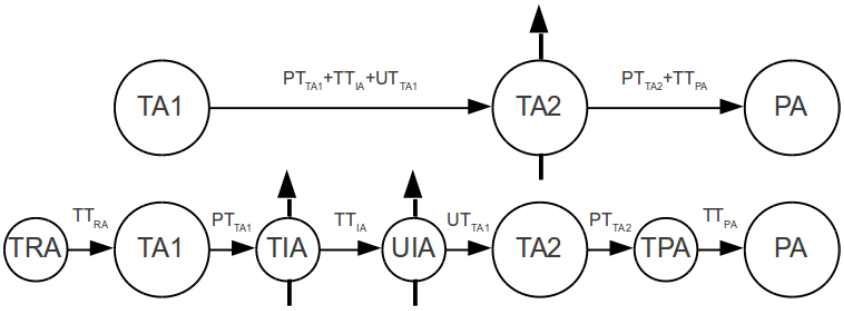

Figure 1: Extended S-graph representation

The standard S-graph representation has the tasks and products as nodes. In this simple example, product *PA* is produced through two consecutive steps *TA1* and *TA2*. The task, whose input needs heating is indicated by an upward arrow, as introduced in Adonyi et. al. (2003). In the extended presentation, additional nodes are added for the transfer of the materials: *TRA* for the transfer of raw material *RA*, *TIA* for the intermediate *IA*, and *TPA* for the product. Additionally, if a material needs heating or cooling, a node is added for the utility stage. In this example only the intermediate needs heating, so an additional node, *UIA* is added to the graph. The weight of the arcs are the time demand of the previous operation, i.e., transfer times (TT_{RA}, TT_{IA}, TT_{PA}), processing times (PT_{TA1}, PT_{TA2}), and time spent on using utility (UT_{IA}).

In each step of the Branch-and-Bound procedure either a processing unit or a heat exchanger is scheduled. In both cases some additional arcs are inserted to the graph. The presence of a processing unit assigned to a task is required from the starting of the transfer of the input materials until the end of the transfer of the output materials. If, for example, a unit is assigned to *TA1*, the schedule arc from the previously assigned task is directed to *TRA* and the schedule arc to the next scheduled task will start from *UIA*.

To illustrate the arcs induced by the scheduling of heat exchangers, two batches of products *PA* and *PB* are considered. The recipe of *PB* is similar to the one of *PA*, except for the intermediate, which needs cooling instead of heating. Suppose that a heat exchanger is assigned to exchange heat between these two intermediates in the first batch, and then it is assigned to exchange heat between the same materials in the second batch. This scheduling decision for the heat exchanger is denoted by the arcs shown on Figure 2. In the case if the transfer of the material *TIB* takes longer time, part of the stream may exchange heat with both batches of *TIA*. This case is represented on Figure 3.

3.3 Interaction between the MILP master problem and the S-graph framework

While the graph is being extended with additional schedule-arcs, the MILP model is also updated. This is carried out by setting the values of the binary variables that has been decided by the decisions made so far.

The S-graph representation of a partial schedule can however provide additional information for the MILP problem as well. As an example, if there is a non-negative directed path from *UIA* to *TIB* because of some scheduling decisions made on processing units, *TIA* and *TIB* will obviously unable to exchange heat. Following this observation, all the corresponding heat exchanger assignment variables, and heat exchanger sequencing variables can be set to 0. In a similar fashion, decisions made on heat exchangers can influence the assignment and sequencing variables of processing units.

The interaction between the modules is not one directional. If an MILP relaxation finds an integer optimal solution, no further branching is needed at that part of the tree. Additionally, the MILP relaxations can be used to provide lower bounds on the time needed for utilities, with which values the weight of the corresponding utility arcs can be increased.

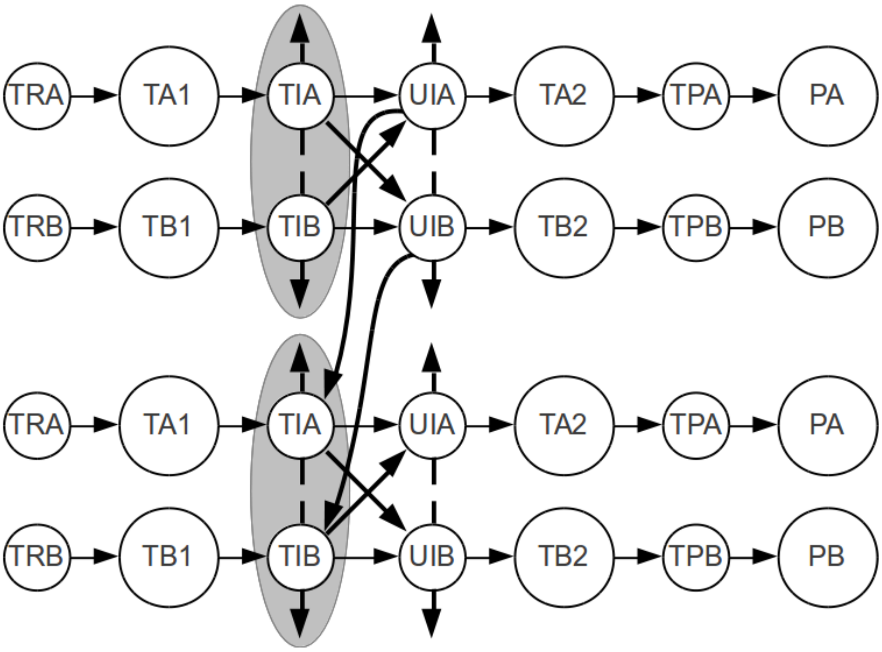

Figure 2: Schedule-arcs for heat exchangers

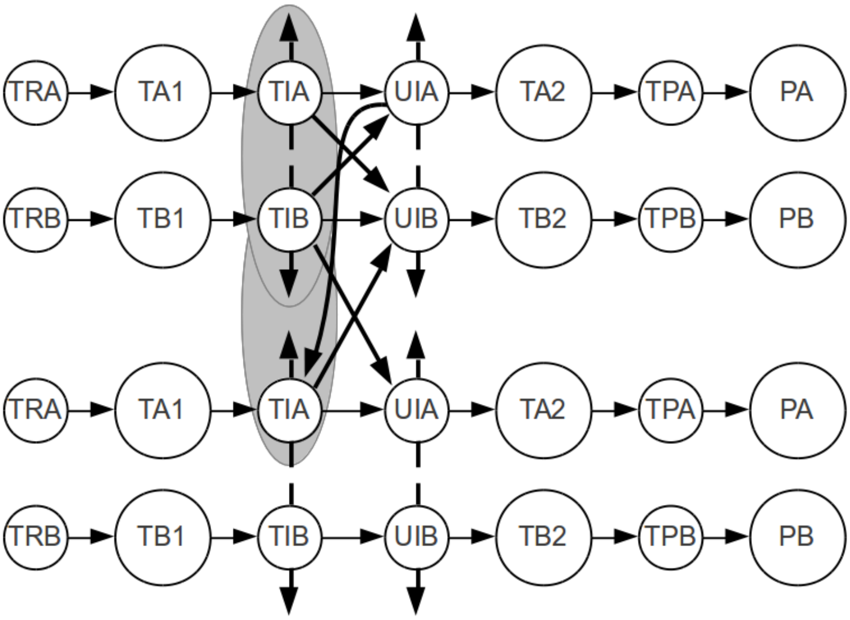

Figure 3: Schedule-arc for one side of the heat exchanger

4. Concluding remarks

A new approach has been presented for the simultaneous scheduling and heat integration for multipurpose batch plants. The proposed approach minimizes the utility usage within a given time horizon applying both MILP programming techniques and the S-graph framework. Unlike the formerly published S-graph based algorithm, this approach considers the scheduling of both heat exchangers and processing units, and allows a stream to exchange heat with several other streams.

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