Exploiting plant and process flexibility at the operational level

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Abstract

Although the synthesis problem is usually posed and solved at the design stage, in some cases, some synthesis decisions remain open and can be easily revised during the plant operation, especially if batch processes are considered. This work proposes the joint resolution of the synthesis and scheduling problems, coupled through a single mixed integer linear programming model (MILP), in order to attain an integrated exploitation of the flexibility exhibited by both, plant and process, leading to improved decision making. Typical process representation models can be extended to also consider synthesis information/decisions, leading to a synthesis state task network (SSTN). The main goal is to obtain the optimal structure determined by the best possible schedule. A case study is successfully solved to illustrate the capabilities of the proposed method.

Keywords: Process Synthesis, Scheduling, dynamic optimization.

1. Introduction

Operations scheduling is a critical issue in batch processes. Mathematical models developed to support this activity typically include decisions of where and when to operate, and seek to minimize the operating time required to follow the process recipe. But scheduling decisions also affect process feasibility, sustainability, safety, etc., and so other objectives can be considered, related to production, environmental impact, etc. In the last decades, there have been significant advances in the application of short-term scheduling methodologies, especially to solve industrial problems. In the literature, we can find many works addressing this decision level (Aguirre (2011), Lima et al. (2011), Floudas and Ling (2004), Kallrath (2002), Kondili et al (1993), etc.). But it should be noted that, in most of these approaches, this optimization is based on previous decisions, typically associated to design and planning tasks.

On the other hand, optimal process synthesis is one of the most challenging problems in Chemical Engineering. Its aim is the identification of the best solution within a flow sheet super structure. The decision making process involves the consideration of different alternatives in the flow chart for carrying out the process of transforming raw materials into finished products. Process synthesis is important not only to identify the more efficient or economic process, but also to improve sub problems such as pollution prevention, freshwater consumption and minimization of energy. Integration of these decisions can be also found in the literature. Floudas (2001) propose a design synthesis scheduling approach to take decisions in the Supply Chain and conclude that the computation capacity is an important parameter to consider when this issue is solved.

Either for solving the process synthesis problem or for solving the scheduling problem, it is essential to have sufficient knowledge of the process, in the sense then available alternatives should be clearly identified in order to solve the problem fulfilling certain
objectives. In particular, reaction synthesis problem is important not only to determine raw material necessities, but also because it constraints the process configuration.

Therefore, this paper proposes a mixed integer linear programming problem (MILP) model that integrates the scheduling problem with some operating decisions which are usually considered as part of the process synthesis problem, with the aim to improve decision making support.

2. Problem statement

2.1 Scheduling problem

The scheduling model originally proposed by Kondilli (1993) has been adopted as a basis for the proposed formulation, and has been complemented with additional constraints, mainly to consider the proper allocation of available equipment to the different tasks. Also the objective function has been modified to minimize the total cost, which in this case will be the production and the fixed and variable cost associated to the use of the different equipments considered by the process recipes.

2.2 Synthesis problem

The objective of process synthesis is the identification of the best solution of a flow sheet super structure, which includes different alternatives. In this kind of synthesis problems, it takes into account different aspects, such as conversion reaction, raw materials, equipment units and generation of sub-products or contaminants.

This work uses the typical consideration of a superstructure of the process. This superstructure is introduced into the scheduling process recipe, then the solution obtained by the model approach consider different equipment options to solve the same operation, the consideration of different equipments is related with the consideration of different costs (fixed/variable) and conversions.

2.4 Synthesis State Task Network

In order to represent plant and process information, it is proposed to extend the STN (State Task Network) representation to include data related to the synthesis decisions to be considered. This extension considers different structures of the process, and contains data related to the process flow diagram when integrated Synthesis and Scheduling decisions have to be taken.

Figure 1a represents the typical synthesis problem that considers different equipment units able to perform the same task in the process flowsheet; Figure 1b shows the STN representation for the scheduling problem that considers the recipe of the process, including states, units and tasks, and figure 1c shows the representation proposed by this work (Synthesis State Task Network) and introduces the synthesis considerations into the STN. Additional aggregated data to be considered include, for example, the different conversions which can be achieved when using different reactors, or the equipment costs (fixed and variable costs).
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Figure 1. Description of the Synthesis State Task Network

3. Case study

This case study is based on the scheduling example proposed by Kondili et al. (1993), and the synthesis problem presented by Grossmann et al. (1996). These cases are widely used in the scheduling and synthesis literature. The problem to be solved involves 5 tasks (heat, reaction 1, reaction 2, reaction 3 and distillation), 9 states (feed A, feed B, feed C, hot A, intermediate AB, intermediate BC, impure C, product 1 and product 2) and 4 equipment units (1 heater, 2 reactors and 1 distiller). The production of the two final products from feedstocks A, B and C are given as follows:

- Task 1: Heat A for 1 hour.
- Task 2: React for 2 hours a mix 50% feed B and 50% feed C, forming intermediate BC.
- Task 3: React for 2 hours a mix 40% hot A and 60% intermediate BC, forming intermediate AB (60%) and product 1 (40%).
- Task 4: React for 2 hours a mix 20% feed C and 80% intermediate AB, forming impure E.
- Task 5: Distill impure E to separate product 2 (90% after 1 hour) and intermediate AB (10%, after 2 hours), which is recycled.
Different equipment units have been considered to perform the different tasks, as indicated in Table 1:

### Table 1. Case Study Equipment units, conversion and costs.

<table>
<thead>
<tr>
<th>Task</th>
<th>Equipment</th>
<th>Conversion</th>
<th>Variable cost</th>
<th>Fixed cost</th>
<th>Operation time</th>
</tr>
</thead>
<tbody>
<tr>
<td>Heat</td>
<td>Heater 1</td>
<td>-</td>
<td>0.4</td>
<td>8</td>
<td>1</td>
</tr>
<tr>
<td></td>
<td>Heater 2</td>
<td>-</td>
<td>0.5</td>
<td>7</td>
<td>1</td>
</tr>
<tr>
<td></td>
<td>Heater 3</td>
<td>-</td>
<td>0.6</td>
<td>6</td>
<td>1</td>
</tr>
<tr>
<td>Reactions 1, 2 and 3</td>
<td>Reactor 1</td>
<td>1.00</td>
<td>1.0</td>
<td>10</td>
<td>1</td>
</tr>
<tr>
<td></td>
<td>Reactor 2</td>
<td>1.00</td>
<td>1.0</td>
<td>10</td>
<td>1</td>
</tr>
<tr>
<td></td>
<td>Reactor 3</td>
<td>0.90</td>
<td>0.9</td>
<td>8</td>
<td>2</td>
</tr>
<tr>
<td></td>
<td>Reactor 4</td>
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<td>0.9</td>
<td>8</td>
<td>2</td>
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<tr>
<td></td>
<td>Reactor 5</td>
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<td>7</td>
<td>2</td>
</tr>
<tr>
<td></td>
<td>Reactor 6</td>
<td>0.85</td>
<td>0.8</td>
<td>7</td>
<td>2</td>
</tr>
<tr>
<td>Distillation</td>
<td>Distiller</td>
<td>-</td>
<td>0.5</td>
<td>10</td>
<td>1</td>
</tr>
</tbody>
</table>

### 4. Case study results

The resolution of the proposed mathematical model provides the optimal assignment of equipment units and the best sequence and timing (Figure 2) regarding the considered objectives. In particular, it is required the installation of the heater 3, the use of reactors 1 and 2 (technology 1), and also reactors 3 and 4 (technology 2) and the distiller. Although the use of these reactors implies higher fixed costs, they also exhibit higher conversion, which is reflected in a reduced requirement of raw materials.

The importance of a joint decision making, including operational and synthesis levels can be assessed through the fact that the optimal result may include the use of more than one of the available reactor technologies in the time horizon.

![Figure 2: Computational results of the proposed case study.](image)
5. Conclusions

This work addresses the integration of the process synthesis decisions with operational decisions, determining the optimal equipment use (task assignment and timing) considering elements typically distributed in different hierarchical decision making levels. The resulting combined problem has been modeled using a MILP-based approach by introducing the use of dynamic programming, obtaining improved solutions in typical scheduling problems.

References


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