Multiobjective optimization of multipurpose batch plants using superequipment class concept

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Abstract

We present a novel approach for solving different design problems related to single products in multipurpose batch plants: the selection of one production line out of several available, additional investment into an existing line or plant, and grass-root design of a new plant. Multiple objectives are considered in these design problems. Pareto-optimal solutions are generated by means of a Tabu Search algorithm. In the novel approach the concept of superequipment has been defined as an abstract model, which is capable of performing any physico-chemical batch operation. Each superequipment is transformed into a real equipment unit, for example a reactor, during or after the optimization in order to evaluate performance parameters of a design. This novel concept uses an implicit definition of a superstructure and essentially optimizes on the transfers between different equipment units. On the basis of two case studies we demonstrate that the application of the superequipment concept offers a number of advantages for the investigated design problems. The comparison with optimization results obtained with a conventional Tabu Search algorithm revealed that the superequipment method identifies the Pareto-optimal solutions in significantly reduced computation time.

Keywords: Tabu Search, multiobjective optimization, batch process, superequipment

1. Introduction

Chemical companies currently face different problems related to the global market changes. In speciality chemicals and pharmaceuticals production customers require smaller amounts of product orders, faster delivery times and on demand production. Some of the tasks which are closely related to industrial problems of batch processing can be solved by help of optimization techniques. Usage of such methods allows for faster screening of production capacities, plant line selection for given product, decision making, planning and assessment related to the plant and process.

Relatively few articles have been presented that assess the optimal design for a single batch process. In the optimization of multipurpose batch plant designs (MPBP), Wellons and Reklaitis (1989, 1991) proposed a MINLP method for scheduling and optimization. Povoa and Macchietto (1993) described the possibilities of using combinatorial optimization for solving design related problems in multipurpose batch plants. Cavin et al. (2004, 2005) presented a Tabu Search algorithm for identifying the optimal design of a single process in a multipurpose batch plant.

We present a novel approach for solving different design problems related to single products in multipurpose batch plants using the concept of superequipment as an abstract model utilizing a virtual unit, which is capable of performing any physico-chemical batch operation. Each superequipment is transformed into a real equipment unit, during or after the optimization in order to evaluate performance parameters of a design. This novel concept will be demonstrated on two case studies.
2. Multipurpose Batch Plant Optimization using Superequipment Class

2.1. Problem Definition
The new approach is used for solving multipurpose batch plant design problems in which is given a chemical recipe (i.e. a series of chemical/physical tasks, the capacity requirements for each task of recipe per unit of final product, the base duration of each task at the input scale, recipe constraints), plant and equipment data (i.e. equipment description including detailed specifications such as e.g. operating T-P ranges), economic data (i.e. detailed cost composition on campaign basis and investment costs where applicable), design heuristics (i.e. which equipment class is capable of performing which recipe operation classes) and one or more objective functions. The objective is to determine a set of Pareto-optimal and structurally diverse layouts for the process, i.e. allocation of recipe tasks to equipment units, structure and order of the final recipe (e.g. in parallel or in series use of units).

2.2. Superequipment
If we think about the retrofit problem of additional investment into an existing plant line, we see that the combinations of equipment on buy list and their characteristics (i.e. unit size, lining material, options, TP range) require exponential solving time. During a standard Tabu Search (TS) optimization it is necessary to generate a number of combinations in form of designs, where the allocation of each new unit should be varied in the design in order to have a good chance of finding the global optimum. Superequipment concept has been developed as alternative approach. It simplifies the combinatorial problem, because one superequipment unit substitutes any unit from the buy list. Superequipment is not a real unit. It stands for a model of a unit, where each piece of superequipment can be transformed into a real apparatus in the final design. In extension of a standard TS approach (see Cavin et al., 2005) the superequipment class S is defined in the way that any operation from the operation classes present in the operation-to-equipment assignment matrix A can be conducted in the superequipment:

\[
S := \bigcup_i A_{i,EqClass}
\]  

(1)

We define a superequipment unit as an unit belonging to the equipment list E:

\[
\text{Superequipment \_unit} := (E.EqClassID = S)
\]  

(2)

Figure 1: Transformation of a superequipment unit into a real equipment unit.
Each piece of superequipment used in a design must be transformed into an existing real unit at some point during the optimization. The superequipment transformation example in Figure 1 shows three operations, where the second operation is conducted in the superequipment (original design). After transformation two possible solutions exist - a reactor (middle design) or an extractor (bottom design). This flexibility in the class type, size, lining material is maintained through the optimization process up to the final results list, so that the decision maker can see all possible proposals.

2.3. Optimization Algorithm Formulation
The method aims at finding the optimal assignment of recipe blocks into given equipment units. The transfers between the units are also determined and define the moves of Tabu Search. As an input, a base case layout and initial batch size, cycle time, operation durations, temperatures, pressures and other data are required. During each iteration one design is altered and all neighbors originating from that particular design are evaluated for their parameters. The design parameters, such as task durations, volume and time requirements for each block are adjusted and scaled accordingly.

The algorithm has been designed for handling multiple objectives, where prioritized optimization objectives can be selected from a list comprising e.g. production rate, number of equipment units in design, batch size, productivity per total nominal volume of significant equipment units used in a design, net present value (NPV) of a project with or without investment and payback period. More details on the algorithm and its mathematical implementation can be found in Cavin et al. (2005).

3. Results of Case Studies and Discussion
The novel concept using superequipment class will be applied to two problems, i.e. investigating possible investment into an existing line and the selection of one production line from a number of available facilities.

3.1. Investment Scenario for an Existing Plant and a Given Recipe
The Vitamin C case study is based on the Reichestein synthesis and was selected for its simplicity to demonstrate the basic principle of superequipment concept. We define a small batch plant (Plant C4) and examine investment possibilities in order to maximize the NPV of a project with investment. There is only space for two additional unit installations within the production building. A comparison of superequipment concept and conventional TS optimization (Cavin et al., 2004, 2005) is presented.

The recipe comprises 8 blocks each consisting of several unit operations. The base plant C4 consists of 5 reactors (1 x 10 m$^3$, 4 x 6.3 m$^3$) and one 1.2 m$^3$ centrifuge. The plants

![Image](82x602)

Figure 2. Investment case study: optimal designs for base plant C4 (left) and plant C4S considering investment as identified with superequipment approach (right).
Table 1: Investment case study using superequipment approach: subset of Pareto-optimal designs.

<table>
<thead>
<tr>
<th>Design rank [#]</th>
<th>Equipment size [m³]</th>
<th>Investment [kUSD]</th>
<th>Productivity [kg/h]</th>
<th>Nr. of units [pcs.]</th>
<th>Payback time [year]</th>
<th>NPV [kUSD]</th>
<th>Campaign time [years]</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 react+centr.</td>
<td>10; 1.2</td>
<td>820</td>
<td>27.8</td>
<td>8</td>
<td>6.6</td>
<td>1300</td>
<td>4.1</td>
</tr>
<tr>
<td>35 centrifuge</td>
<td>1.2</td>
<td>340</td>
<td>23.1</td>
<td>7</td>
<td>12.5</td>
<td>1130</td>
<td>4.9</td>
</tr>
<tr>
<td>49 react.+cryst.</td>
<td>16; 6.3</td>
<td>800</td>
<td>21.3</td>
<td>8</td>
<td>7.2</td>
<td>1180</td>
<td>5.4</td>
</tr>
</tbody>
</table>

C4r, C4ce and C4rce used for conventional optimization have one 10 m³ reactor, one 1.2 m³ centrifuge, or both units in addition to the base plant, respectively. The plant C4S consists of the base plant plus two superequipment units that can be transformed into reactors or centrifuges.

For the base plant (Plant C4) the optimal production rate is 20.2 kg/h when implementing a design with 6 equipment units (see Figure 2 left). In examining possible investment options two superequipment units are added to this plant, resulting in designs with zero, one or two superequipments in addition to the units from plant C4. A selection of feasible investment options is listed in Table 1, where the designs are Pareto-optimal in the listed objective functions. The best design according to productivity and NPV utilizes additionally one 10 m³ reactor and one 1.2 m³ centrifuge (see Figure 2 right). Objective function values are: productivity 27.8 kg/h, batch size 0.24 t/batch, and payback time of 6.6 years. Cycle time is reduced from 730 min to 525 min by better utilizing the equipment and parallel assignment of the two centrifuges.

For the standard optimization the mean CPU time required for finding the apparent global optimum, i.e. the best value found in a specified number of runs, was 3510 s. The superequipment method requires on average 2430 s; here the problem is less constrained and requires less iterations to reach the apparent global optimum. Furthermore the superequipment approach has the significant advantage that only the maximum number of additional units has to be specified for the investment scenario while an explicit definition of a larger number of equipment is required in the conventional approach.

3.2. Plant Selection for given Recipe

This case study shows production of a fine chemical used in the pharmaceutical and photo industry. The synthesis is based on a reactant known under commercial name Quinaldine. The recipe and basic process simulation of 4-(2-quinolinylmethoxy)-phenol, referred to as product H, have been presented by Petrides et al. (2002). The aim is to show how in a single run diverse plant lines can be optimized by means of superequipment method and can be compared with each other.

The recipe comprises 12 blocks each consisting of several unit operations. Three production lines are available: C10 (8 reactors of different size, 4 centrifuges, 4 filters, 0 crystallization units), Q2 (11 / 2 / 3 / 2), and C11 (21 / 8 / 9 / 5). The superequipment plant consists of 24 superequipments to be transformed into equipment from each line. Table 2 provides a comparison of parameters of designs mapped completely to the three plant lines. Design #3 is the overall best in terms of productivity. This is also the best design found for plant C11. The large number of 24 units used for production implies increased costs for this design (NPV=23.0 mio. USD) and thus not reaching the optimum for the NPV. This design is actually performing all recipe blocks in parallel and thus creating overhead in cleaning and labour demand. The productivity per total nominal volume of significant equipment is low (0.71 kg/(h m³)).
Table 2: Plant selection case study: subset of designs as obtained with superequipment approach sorted according to productivity. Plant line IDs 1, 2 and 3 refer to lines C10, Q2, and C11, respectively. Bold numbers indicate optimal productivity in each line.

<table>
<thead>
<tr>
<th>Design ID</th>
<th>Plant line ID</th>
<th>Prod. rate</th>
<th>Batch size</th>
<th>Nr. equip.</th>
<th>NPV [mio. USD]</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>3</td>
<td>135.1</td>
<td>1.27</td>
<td>24</td>
<td>23.0</td>
</tr>
<tr>
<td>7</td>
<td>3</td>
<td>133.0</td>
<td>1.24</td>
<td>21</td>
<td>22.8</td>
</tr>
<tr>
<td>1</td>
<td>1</td>
<td>130.9</td>
<td>1.60</td>
<td>13</td>
<td>23.3</td>
</tr>
<tr>
<td>4</td>
<td>1</td>
<td>130.9</td>
<td>1.60</td>
<td>14</td>
<td>23.2</td>
</tr>
<tr>
<td>1</td>
<td>3</td>
<td>90.3</td>
<td>0.97</td>
<td>13</td>
<td>22.1</td>
</tr>
<tr>
<td>2</td>
<td>2</td>
<td>74.0</td>
<td>0.69</td>
<td>13</td>
<td>21.0</td>
</tr>
<tr>
<td>4</td>
<td>2</td>
<td>68.8</td>
<td>0.63</td>
<td>14</td>
<td>20.6</td>
</tr>
<tr>
<td>1</td>
<td>2</td>
<td>58.4</td>
<td>0.63</td>
<td>13</td>
<td>19.3</td>
</tr>
</tbody>
</table>

The best productivity in the plant C10 can be achieved by design #1 being only 3% less effective than design #3, but it utilizes only 13 units, reducing the costs and reaching the optimum in NPV equal to 23.3 mio. USD for the whole campaign. Plant Q2 is dedicated for small productions and has no 10 m³ reactor, therefore the best achievable productivity is 74.0 kg/h with design #2. All of the resulting Net Present Values are rather similar, because of the high fraction of raw material and solvent costs. Thus the primary criteria for decision might be for example productivity, number of units used or batch size. If the campaign time is the main issue, design #3 should be implemented in plant C11. On the contrary, if the free capacity of a big plant (plant C11) was required for upcoming campaigns, design #1 in plant C10 could be a good compromise between performance, NPV and number of units used while keeping the large plant free.

Note that the same design can have multiple instances in the results table. Since the equipment units differ in each plant, the performance indicators also differ. Figure 3 shows the relationships of productivity vs. number of used equipment units for the three plants. A subset of designs with best productivity for given number of units and given plant is displayed. A minimal number of 9 units is needed to process the 12 recipe blocks. The maximal number is 24 (design #3). The design #3 can be matched only with plant C11 without additional investment. The mapped designs show a trend of increasing productivity with increasing number of equipment. The best designs with 15 equipment units (Figure 3) do not include two centrifuges in parallel mode as in the best designs with 14 units. This increases the cycle time. If a design with 15 units and two parallel centrifuges is mapped into plant C10 or plant C11, an additional reactor (as compared to the best design with 14 units), which is placed in series with another reactor, becomes the volume bottleneck and no bigger unit is available.

In the plant Q2, the apparent global optimum, i.e. the best value found in a specified number of runs, with 74.0 kg/h and 13 units has not been found with the conventional TS method (200 iterations without finding an apparent global optimum and 40 restarts requiring ca. 230 minutes). This can be explained by too constrained searching space and neighborhood, where the only possibility of diversification in current implementation of TS is in the restarts. However, superequipment method is less constrained due to the "chameleon" property of each unit and the diversification process is ensured naturally by moving through the solution space almost without limits.
Figure 3: Plant selection case study: productivity vs. number of equipment units after matching superequipment designs to plants C10, Q2 and C11. Designs with maximal productivity for a given number of units are displayed. Designs #1-3 refer to Table 2.

In total 26009 s were needed to optimize the three plants with the standard TS while the superequipment plant optimization with 24 units and three lines required 11340 s. Again the superequipment concept offered practical advantages and reduced computation time.

4. Conclusions

In the novel approach the concept of superequipment has been defined as an abstract model, which is capable of performing any physico-chemical operation. Each superequipment is transformed into a real equipment unit, for example a reactor, during or after the optimization in order to evaluate performance parameters of a design. Corresponding transformation heuristics need to be defined for each problem type. For different fields of application the superequipment concept means a considerable saving in computation time and effort because the optimization problems are reduced in size, repetitive optimization runs are avoided and the search space is less constrained.

References