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Optimization of chemical industrial enterprises' problems using mixed integer programming

Theses

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1. Introduction

My thesis deals with optimization problems. These problems are often approached using mathematical programming, but sometimes, when the problem is too complex or its size is too large, application of mathematical programming only does not lead to results.

My goal during my research work was to prove that mathematical programming can be an effective tool when solving practical problems, if its efficiency is improved using some advanced techniques. In these cases, I have tried to improve the solvability through three different ways: 1) modifying the solution algorithm; 2) developing a new, simplified the superstructure; 3) applying decomposition strategy.

2. Literature overview

2.1. Optimal design of distillation systems

In order to separate a liquid mixture into its components, multistage or fractionated distillation is applied in the industry. Distillation systems handle large material amount thus they have huge investment- and energy demands. By rational design, it is possible to save considerable expenses, thus process optimization has serious significance in this area. With the development of operation research tools, trials aiming optimal design started, by which the optimal reflux ratio and number of stages is determined for reaching a certain separation level.

Since the number of stages, which can take only integer values, also has to be decided, integer variables must be used when modeling these processes. Describing phase equilibrium and component balances requires applying nonlinear constraints. Consequently rigorous modeling of distillation columns needs solution of Mixed-Integer Nonlinear Programs (MINLPs).

Farkas[1] developed a new distillation column superstructure and an MINLP representation. The new model excludes the possibility of structural redundancy already at the level of the superstructure, thus reducing numerical problems. The new superstructure was built up keeping an eye on the principle of the binarily minimal representation.

Besides advances in modeling techniques, emphasis has been laid on the improvement of effectiveness of solution algorithms. The Outer Approximation (OA) algorithm originally developed by Duran and Grossmann[2] and its logic based variant, see Bergamini et al.[3] has been

[1] Farkas, T. (2006) Chemical Process Synthesis Using Mixed Integer Nonlinear Programming, PhD Thesis, Budapest University of Technology and Economics

[2] Duran, M. A.; Grossmann, I. E. (1986) An outer-approximation algorithm for a class of mixed integer nonlinear programs. Mathematical Programming, 1986, 36, 307-339.

[3] Bergamini, M. L.; Aguirre, P.; Grossmann, I. E. (2005) Logic based outer approximation for global optimization of synthesis of process networks. Computers and Chemical Engineering, 2005, 29, 1914-1933.

modified several times by different research groups. The aim of these modifications was to ensure finding the global optimum. Thus Bergamini et al.[4] performed a piecewise estimation of nonconvex or bilinear constraints. Solution of MILP masterproblems was not continued until finding global optimum, only while getting a better solution than the current one.

While there have been impressing advances in the area, still there are remaining possibilities for developing new models and algorithms. It can generally be observed, for example, that the solver often has to face difficulties due to strong nonlinearities. After a certain number of constraints, the solution becomes impossible without providing good initial values for the variables, thereby reducing the initial infeasibility. During my research work, I aimed to develop a modified OA algorithm that calculates initial values for each variable using the binary vector provided by the preceding MILP masterproblem. The issue of cutting off possible optimum by linearly approximating nonconvex functions is also needed to be addressed.

2.2. Process scheduling

Process scheduling problems usually involve a diverse data structure. (1) A set of different product orders are considered with specified amount to be produced before their deadlines. (2) A set of different raw materials with release time and amount data can be applied to satisfy the product orders. (3) A set of tasks, i.e. single activities consuming raw materials or intermediates and producing intermediates or end-products constitute the technology used in the production, together with (4) processing time etc. data in the production recipes. (One production recipe contains the characteristics of one task.) (5) A process recipe contains data about the process itself, i.e. relations and connections between tasks. (6) Plant specifications contain information about the characteristics of available processing units and storage tanks, and the allowed connections between them. (7) Detailed technological constraints can be derived from the above data (capacity, storage restrictions etc.). The goal is to find either a solution optimizing objective function (makespan, etc.), or a feasible solution that satisfies the constraints.

Research of process scheduling problems has received ever increasing attention in the past fifteen years. The research aims chiefly application of mathematical programming. Several MILP models have been developed by different research groups, amongst which employing discrete[5], general[6], and unit specific[7] continuous time representations can be found.

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[4] Bergamini, M. L.; Grossmann, I. E.; Scenna, N.; Aguirre, P. (2008) An improved piecewise outer-approximation algorithm for the global optimization of MINLP models involving concave and bilinear terms. Computers and Chemical Engineering, 2008, 32, 477-493.
[5] Kondili, E.; Pantelides, C. C.; Sargent, R. W. H. (1993) A general algorithm for short-term scheduling of batch operations – 1. MILP formulation. Computers and Chemical Engineering. 1993, 17, 211-227.
[6] Maravelias, C. T.; Grossmann, I. E. (2003) New General Continuous-Time State-Task Network Formulation for Short-Term Scheduling of Multipurpose Batch Plants. Industrial and Engineering Chemistry Research. 2003, 42, 3056-3074.
[7] Shaik, M. A.; Floudas, C. A. (2007) Improved Unit-Specific Event-Based Continuous-Time Model for Short-Term Scheduling of Continuous Processes: Rigorous Treatment of Storage Requirements. Industrial and Engineering Chemistry Research. 2007, 46, 1764-1779.

There are some important problems, mainly in the chemical, biochemical, and food industries, where the equipment units have to be connected to each other during the whole duration of an operation. It is also a frequent restriction that an equipment unit can be connected to only one other unit at the same time. This results in a scheduling problem where complicated relations exist between the starting and finishing times of operations. These specific characteristics cannot be handled effectively using the literature representations[5-7]; therefore during my research work, I aimed to develop a new model that directly handles the connections between operations. I have modified the superstructure in such a way that the combinatorial complexity of the problem can be reduced.

In case of industrial scale scheduling problems the number of discrete variables and constraints causes combinatorial difficulties such that finding not only the optimal but even feasible solutions is very hard. In order to deal with industrial scale problems, an abundant number of decomposition approaches have been developed to enhance the efficiency of the models. Three types of decomposition exist: those that can be decomposed are 1) time, 2) units, and 3) tasks/resources.

The most widely studied decomposition method is the first one, which decomposes the problem into several subproblems along the time axis and solves them by an iterative way. The time horizon intervals do not overlap with each other; production amounts of each product are assigned to each time interval by the solution of an aggregated planning model. In the first iteration a subproblem is solved over the first part of the horizon, while a remaining portion of the horizon is modeled in an aggregated way. In the next iteration the solution belonging to the preceding part of the horizon is fixed, and the next portion is solved in details. The actual detailed portion of the horizon is rolling in time, therefore this kind of decomposition method is called “rolling horizon”. The subproblems, being smaller than the original one, are less difficult to solve and it is possible to obtain an optimal solution for them. However, the detailed solution built from them may not be proven optimal. This kind of decomposition strategy has been applied several times in the literature.[8,9]

All these decomposition algorithms share the common disadvantage that the aggregate planning model, which is used to set up production goals in the subproblems, generally overestimates the plant capacity, causing infeasibility in the scheduling phase that determines the sequence and size of the operations. This is particularly true when tight deadlines are present and the plant has to work with its capacity fully utilized.

My goal was to develop a new decomposition based approach which exploits the special structure of the previously developed superstructure. The number of available operations is distributed over

[8] Bassett, M. H.; Pekny, J. F.; Reklaitis, G. V. (1996) Decomposition techniques for the solution of large-scale scheduling problems. AICHE Journal. 1996, 42, 3373-3387.

[9] Wu, D.; Ierapetritou, M. G. (2003) Decomposition approaches for the efficient solution of short-term scheduling problems. Computers and Chemical Engineering. 2003, 27, 1261-1276.

a number of MILP subproblems. Thus the subproblems have smaller size, being able to find good solution in reasonable time.

3. Methods

The modified Outer Approximation algorithm was implemented in AIMMS 3.7 model developing system. AIMMS includes a C++ based GMP function library[10], using which the algorithm can be built and modified easily, allowing the user to develop his/her own solver. I have used this function library during my research work.

The new MILP model for optimizing scheduling problems with special characteristics, and the Rolling Operation decomposition algorithm have also been implemented in AIMMS 3.7 model developing system. CPLEX 10.0 was used as MILP solver.

4. Results

4.1. Modified OA algorithm for optimizing extractive distillation structures

The scheme of the modified Outer Approximation algorithm can be seen in Figure 1.

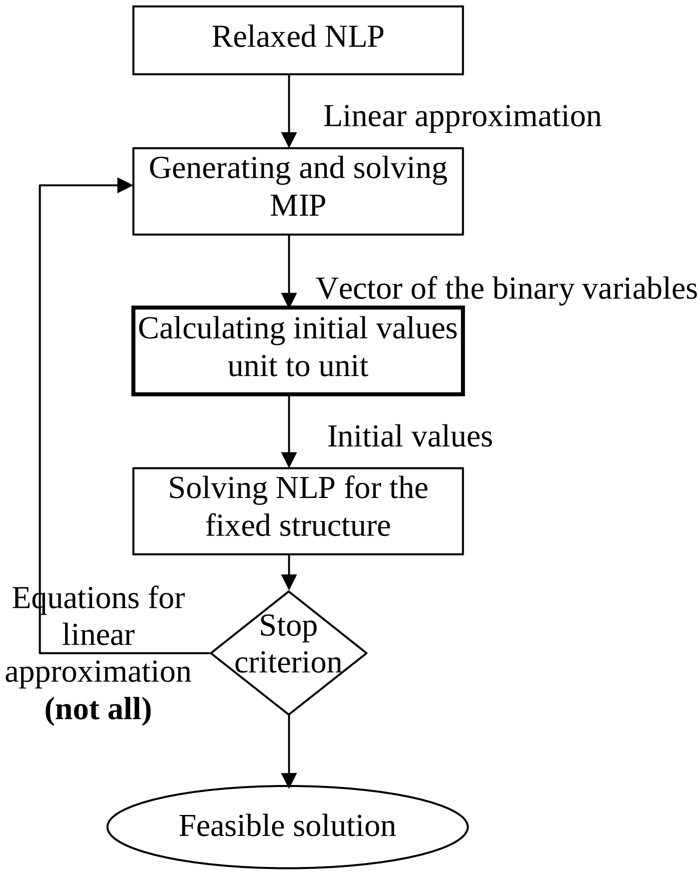

Figure 1. Modified Outer Approximation algorithm

[10] Bisschop, J.; Roelofs, M. (2007) AIMMS. The Language Reference. Paragon Decision Technology, Haarlem, The Netherlands.

The modified Outer Approximation algorithm has been tested using a complex extractive distillation problem. Our goal is to separate a three-component methanol-ethanol-water mixture into its components through extractive distillation. We have three possibilities: either we can use heavy solvent (i.e. ethylene glycol) fed into the column above the feed; or we can use light solvent (i.e. methanol) fed into the column below the feed; or we can use both of them simultaneously. By combining the different process variants, the superstructure presented in Figure 2 is constructed.

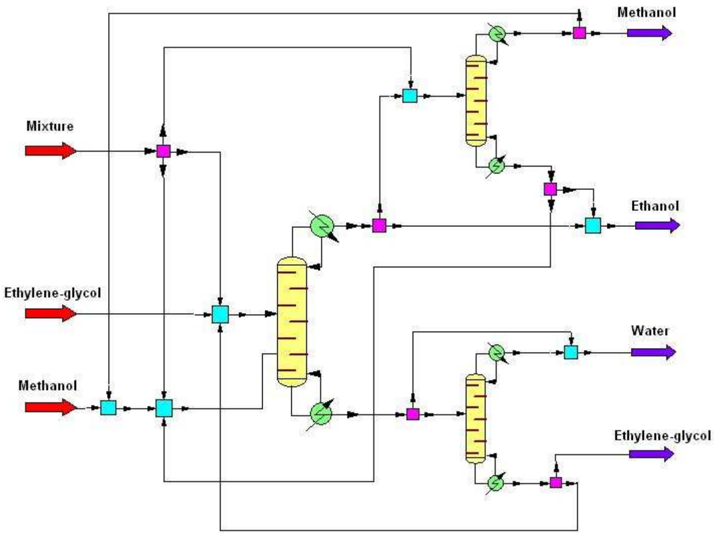

Figure 2. Superstructure of the testproblem

The limit number of iterations is set to ten; the solution time is 3917 sec, i.e. approximately one hour. The individual NLP-s require 10-30 sec, due to the good initial values. The calculation of initial values requires 1-3 sec in each iteration. The obtained solution structure applies glycol as entrainer; the extractive column contains ten stages, the conventional column used for separating the methanol / ethanol mixture and for separating the water / glycol mixture consists of twenty-five and eight stages, respectively.

In the new algorithm, not all the nonlinear equations are used for the linear approximation in the MILP masterproblem. Those that are used for modeling phase equilibrium are omitted. As a result, the value of the objective function is lower than the one with the original algorithm, and the solution time increases less steeply. This results in a total solution time shorter by 75 %, as it is shown in Table 1.

Table 1. Solution data with the modified algorithm

	Objective function	Solution time [CPU sec]
Original	185.12	15270
Modified	183.96	3917

4.2. New MILP model and decomposition algorithm for solving complex scheduling problems

The new MILP model for optimizing scheduling problems with special characteristics was tested using an existing problem in the beer industry. The technological scheme can be seen in Figure 3. The example contains seven equipment units and two products.

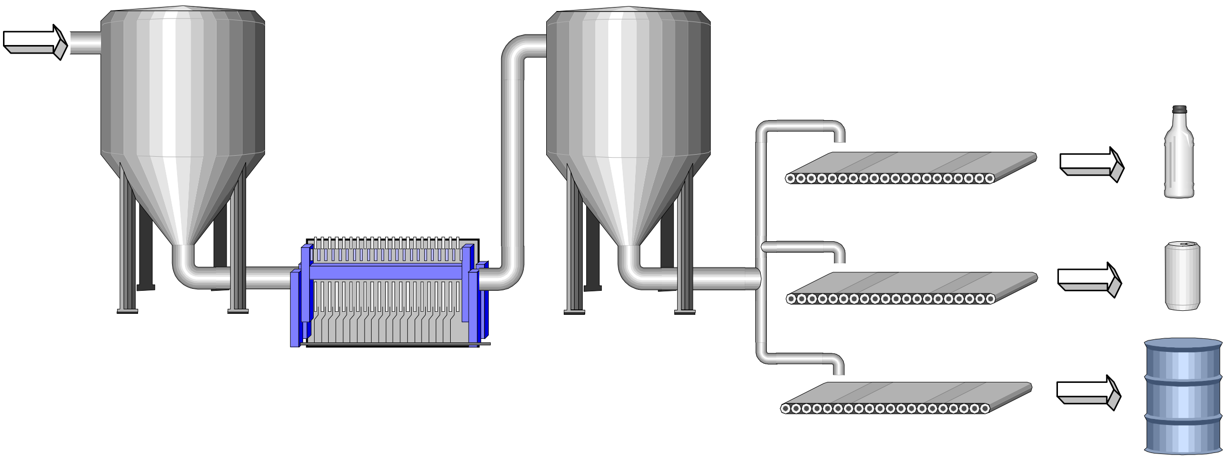

Figure 3. Flowsheet of the industrial problem

Table 2. Solution data with the new model

New model		
nr. of operations	Objective function	Solution time [CPU sec]
6-1-4	28.600	2.95
3-2-1	25.000	1.75
3-2-2	23.250	4.74

The objective function values and solution times are presented in Table 2. The solution schedule can be seen in Figure 4. The solution times are shorter by several orders of magnitude than those of previously modified literature models.

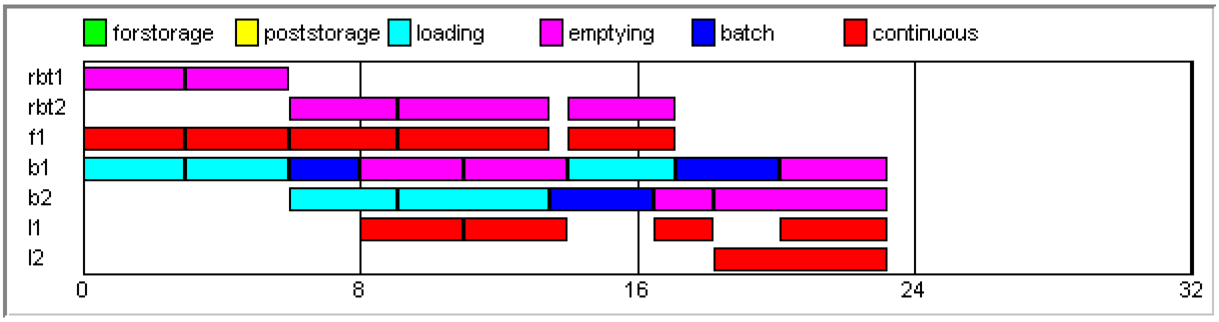

Figure 4. Solution schedule

The new model had been applied to a middle-sized industrial problem containing 34 equipment units and 24 product orders. At this size the problem is practically unsolvable. Therefore the newly developed Rolling Operation algorithm was applied for solving it. The scheme of the Rolling Operation algorithm can be seen in Figure 5.

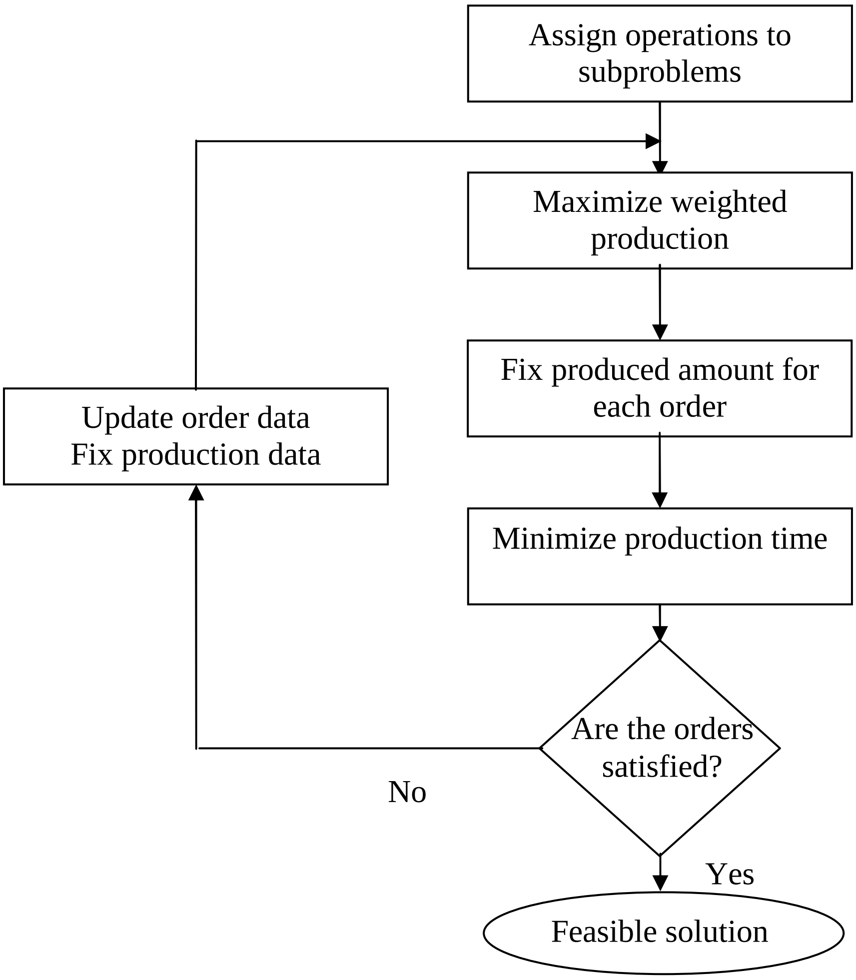

Figure 5. Scheme of the Rolling Operation algorithm

The available number of operation was distributed over a number of subproblems such that they are of an easily solvable size. The subproblems were solved in an iterative way; first the production quantity was maximized, then the production time needed for producing the above quantity was minimized. The solution required 195 seconds altogether; the solution schedule can be seen in Figure 6.

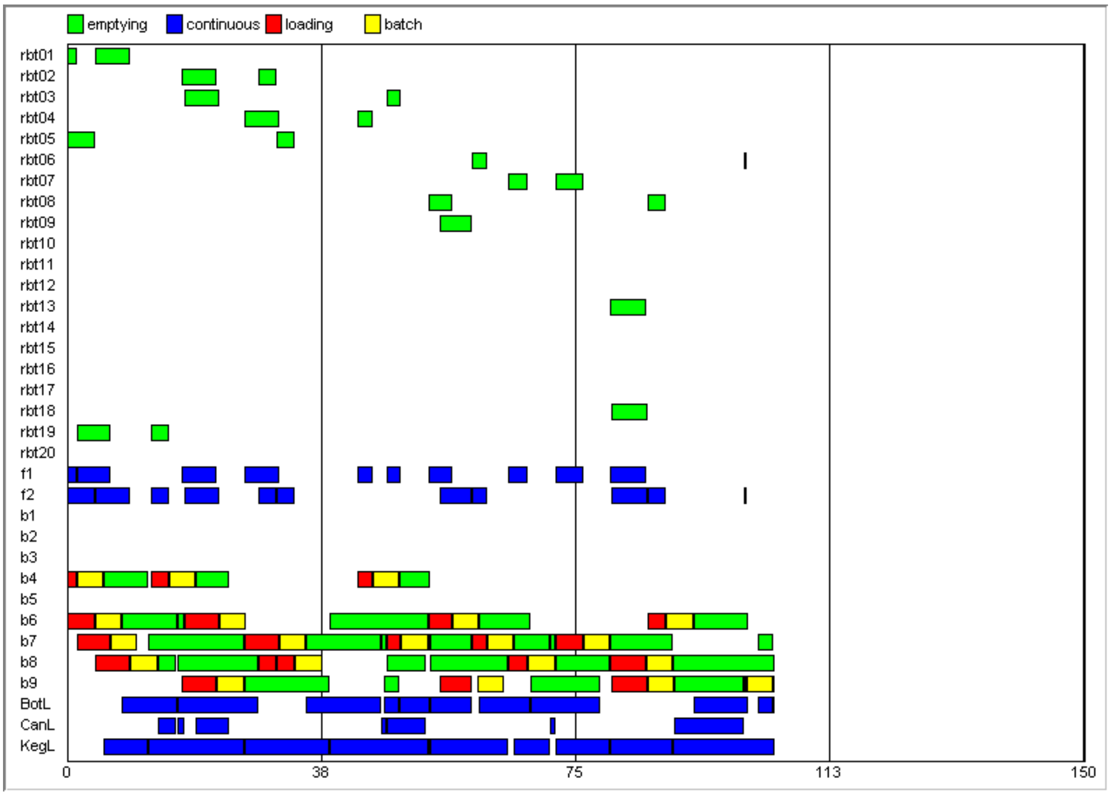

Figure 6. Solution schedule of the industrial problem

5. Theses

I. Thesis. The original Outer Approximation algorithm has been modified in order to make it more suitable to handle complex distillation systems.

a. Inserting a new step, initial values are calculated in each of the iterations for all continuous variables tray by tray, using the binary vector provided by the MILP masterproblems. The initial values, by reducing initial infeasibility, have made it possible for the NLP solver to find feasible solution.

b. The modified algorithm does not use the equations calculating phase equilibrium for linear approximation when generating the MILP masterproblems. It is possible to omit them, because the component balances are sufficient to estimate the composition. Eliminating the nonconvex constraints in the linear approximation step ceases the chance to cut-off feasible solutions from the feasible region. Omitting the strongly nonlinear constraints improves solution quality and reduces solution time. [1, 6, 8]

II. Thesis. I found that traditional literature models are unable to handle some important scheduling problems, mainly in the food industries, which contain storage time constraints, continuous tasks and special connection restrictions between equipment units. Therefore I have developed a new superstructure and MILP model that is more adapted to this kind of problem. The new model directly handles the connections between operations. Reduction of superstructure has been necessary in order to solve the problem, still avoiding cutting off potential optimal solutions. The reduced number of binary variables made the model easy to solve. The new model does not outperform literature models when solving traditional literature problems, but with increasing complexity, its advantages are clearly shown. When solving the studied problem, the solution time is shorter by several orders of magnitude than that of the best literature model. [2, 4, 7]

III. Thesis. In order to solve a real-sized problem from the beer industry, I developed a new decomposition algorithm to handle the combinatorial issues arising from its size. Exploiting the special superstructure, the original problem has been split to several subproblems, by distributing the number of available operations. The subproblems have had smaller size thus being more easily solvable. The algorithm, in each iteration, first maximizes the production quantity, and then minimizes the production time needed for that production quantity. The sum of the solution times of individual subproblems remained fairly short.

If the size of operations is fixed between the two steps, the computation time is shorter; while if only the total production is between those two steps, thus the solution can be largely rearranged, better solution is obtained in longer computation time. The algorithm works reliably even in case of tightened deadlines. The solution can be further improved using a local search procedure. [3, 5]

6. Applications

The modified Outer Approximation algorithm has been employed for solving real sized, complex extractive distillation problems. The shortened – approximately one hour – solution time made it possible to solve in series many optimization problems that differ from each other only in the value of cost factors, during reasonable time. Thus we have been able to study the effect of cost factors on the optimal structure. The obtained results have been published in [10].

The applicability of the new MILP model and Rolling Operation algorithm for real sized industrial scheduling problems is still the objective of intense and fruitful research. The principle of the new algorithm has been used for other food industry problems as well.

7. Publications

Articles that are connected to the thesis:

1. Farkas Tivadar, **Czuczai Barbara**, Rév Endre, Lelkes Zoltán: New MINLP Model and Modified Outer Approximation algorithm for distillation column synthesis. *Industrial & Engineering Chemistry Research*, **2008**, *47*, 3088-3103. (IF(2008): 1,895; I: 1)

2. **Czuczai Barbara**, Farkas Tivadar, Rév Endre, Lelkes Zoltán: New MILP model for solving scheduling problems with special characteristics, *Industrial & Engineering Chemistry Research*, **2009**, *48*, 5321-5335. (IF(2008): 1,895)

3. **Czuczai Barbara**, Farkas Tivadar, Rév Endre, Lelkes Zoltán: Rolling Operation Algorithm for Solving Complex Scheduling Problems, *Industrial & Engineering Chemistry Research*, **2009**, *48*, 3898-3908. (IF(2008): 1,895)

Conference abstracts that are connected to the thesis:

4. **Czuczai Barbara**, Farkas Tivadar, Lelkes Zoltán, Rév Endre: Speciális ütemezési feladatok osztályba sorolása és megoldása. Veszprém, 25-27 April 2007

5. **Czuczai Barbara**, Farkas Tivadar, Lelkes Zoltán, Rév Endre: Rolling Operation dekompozíciós stratégia alkalmazása ipari ütemezési problémák megoldására. Veszprém, 22-24 April 2008

6. Farkas Tivadar, **Czuczai Barbara**, Rév Endre, Lelkes Zoltán: Modified Outer Approximation Algorithm to Optimize Complex Distillation Structure. Veszprém, 15-18 December 2008

7. **Czuczai Barbara**: Speciális jellemzőkkel bíró ütemezési problémák osztályba sorolása és megoldási lehetőségeiknek vizsgálata. Budapest, BME-VBK Doktoráns konferencia, 9 February 2007

8. **Czuczai Barbara**, Farkas Tivadar, Rév Endre, Lelkes Zoltán: Modified outer approximation algorithm for optimizing complex distillation processes. ESCAPE-18, Lyon, 1-4 June 2008

Other articles:

9. Abdulfatah M. Emhamed, **Czuczai Barbara**, Horváth László, Rév Endre, Lelkes Zoltán: Optimization of Desalination Location Problem Using MILP. *AICHE Journal*, **2007**, *53*, 2367-2383.

10. Abdulfatah M. Emhamed, **Czuczai Barbara**, Rév Endre, Lelkes Zoltán: Analysis of Extractive Distillation with Mathematical Programming. *Industrial & Engineering Chemistry Research*, **2008**, *47*, 9983–9995.

Other abstracts where the nominee is presented as an author:

11. **Czuczai Barbara**, Farkas Tivadar, Rév Endre, Fonyó Zsolt, Lelkes Zoltán: Desztillációs kolonna R-gráf alapú szuperstruktúrája és MINLP modellje. Műszaki Kémiai Napok, Veszprém, 2005. April 26.

12. **Czuczai Barbara**, Farkas Tivadar, Rév Endre, Fonyó Zsolt, Lelkes Zoltán: Desztillációs kolonna R-gráf alapú szuperstruktúrája és MINLP modellje. Alkalmazott Informatika Konferencia, Kaposvár, 27 May 2005

13. Abdulfatah M. Emhamed, **Czuczai Barbara**, Horváth László, Rév Endre, Lelkes Zoltán: Desalination location model using mixed-integer linear programming. CHISA-17, Prague, 27-31 August 2006

14. Abdulfatah M. Emhamed, **Czuczai Barbara**, Horváth László, Rév Endre, Lelkes Zoltán: An Improved Desalination Location Model Using Mixed-Integer Linear Programming. Sebha, Libya, 14-16 November 2006

15. Farkas Tivadar, Rév Endre, **Czuczai Barbara**, Fonyó Zsolt, Lelkes Zoltán: R-graph-based distillation column superstructure and MINLP model. ESCAPE-15, Barcelona, Computer Aided Chemical Engineering, Volume 20, Part 1, 2005, Pages 889-894.

16. Abdulfatah M. Emhamed, **Czuczai Barbara**, Farkas Tivadar, Rév Endre, Lelkes Zoltán: Studying extractive distillation processes using optimization. Lyon, 1-4 June 2008