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Logic Based Algorithms for the Rigorous Design of Thermally Coupled Distillation Sequences.

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Abstract

This paper presents an algorithm for the rigorous design of thermally coupled distillation sequences using process simulators. First we show that the two side streams connections that produce a thermal 'couple' can be substituted by a combination of a material stream and a heat flow. In this way, the sequence of thermally coupled distillation columns can be simulated without recycle streams.
The problem can be divided in two levels. An upper level that basically deal with the existence or not of a given distillation column and a lower level dealing with the parameters of an existing columns (number of trays, feed tray position and operational conditions). Therefore, the problem is solved using logic based decomposition algorithm that takes advantage of the structure of the problem iterating between those levels.

Keywords Disjunctive Programming; Distillation; Thermally Coupled Distillation. Process Simulators. MINLP

1. Introduction

Generalized Disjunctive Programming (GDP) is becoming increasingly popular as a solution technique for optimization problems involving discrete decisions, and it has been widely applied in design or retrofit of chemical processes.

However, when a mathematical programming approach is used to synthesize a chemical process usually rely on shortcut or aggregated models in an attempt of capturing the essential of the model while the problem is maintained in a tractable size. This is especially true in the case of distillation systems in which the number of equations involved is large. However, under some situations the shortcut models are not accurate enough and important deviations are produced from the actual behavior.
During the last years have been developed models for the economic design of distillation sequences using rigorous models. However, the high degree of nonlinearity and the difficulty of solving the corresponding optimization models have prevented methods with rigorous models from becoming tools that can be widely used, except by some specialized researchers [1] On another side, modular process simulators include robust and reliable models with special tailored algorithms to each process unit (specially distillation columns) including specialized initialization procedures. In this work, we present a superstructure based algorithm that combine the capabilities of distillation models in modular process simulators – taking advantage of the tailored algorithms designed for distillation and property estimation implemented in these simulators- and logic based Generalized Disjunctive Programming algorithms .

2. GDP algorithm for the design of thermally coupled distillation

2.1. Implementation of the superstructure in a chemical process simulator.

One of the major problems when dealing with thermally coupled distillation sequences in a modular simulator is that the two side streams ‘coupling’ two different columns introduce a large number of recycle streams that are either converged by the simulators or in the optimization stage. In any case these recycle streams considerably slow down the optimization. However, as noted by Carlberg and Westerberg [2] the two side streams connections can be substituted by a single super-heated or sub-cooled stream (depending on it is a net distillate or bottoms stream). In this way, the sequence of thermally coupled distillation columns can be simulated without recycle streams. Consider, for example, Figure 1a. According with Carlberg and Westerberg [2] the liquid and vapor streams of this rectifying section can be substituted by a single superheated vapor stream with a flow equal to the difference between the vapor and liquid streams. The degree of superheating can be easily calculated by an energy balance. In the same way the two streams ‘coupling’ a stripping section of a column with another one can be simulated by a single sub-cooled stream. The major difficulty with this approach is that the degree of superheating (sub-cooling) can be very large producing results without physical meaning that

finish with error messages in the process simulator (i.e. Temperatures under the absolute zero!).
However, in the philosophy of the Carlberg and Westerberg approach it is still possible simulate a thermally couple distillation without recycles by changing the two side connection by a combination of a material and an energy stream. The material stream is vapor at its dew point or liquid at its bubble point depending on where it comes from (a rectifying or a stripping section) and the flow is the difference between the original vapor and liquid streams. Let us go back to Figure 1. If we include a partial condenser (Figure 1b) to provide reflux to the first column then the heat removed in this condenser is exactly the extra heat that must be provided to the second column to simulate the behavior of the two side streams –It is the extra heat that appeared in the energy balance we commented above-.

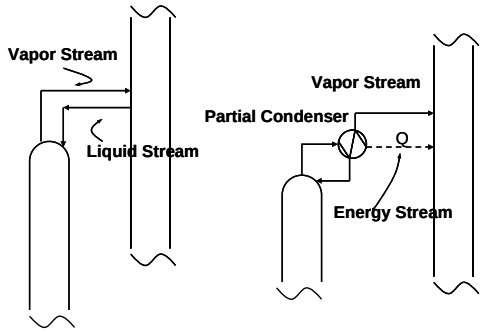

Figure 1. The two side streams coupling two columns can be substituted, at simulation effects, by a material and an energy streams.

Note that this heat exchanger does not really exist but is only an artifice to simulate the behavior of the Thermally Coupled System. By a similar reasoning, the two side streams 'coupling' a stripping section with another column can be simulated by introducing a reboiler and removing from the second column exactly the same heat introduced in the reboiler. It is worth mentioning that in previous reasoning we have assumed that liquid and vapor streams are in equilibrium, and this is no generally the case. But if the vapor and liquid streams are introduced (withdraw) in/from the same tray the error introduced is small and can be neglected.
We use a compact superstructure [3] in which the specific separation task of each column is sequence dependent (Figure 2). In this problem we have decisions at two levels: column level in which we have to decide the number of trays, the feed tray and the operational parameters of each separation in each column and structural level in which we have to decide the existence or not of a given distillation column. The superstructure was set in HYSYS.Plant and the existence or not of a given distillation column was dynamically decided during the optimization process.

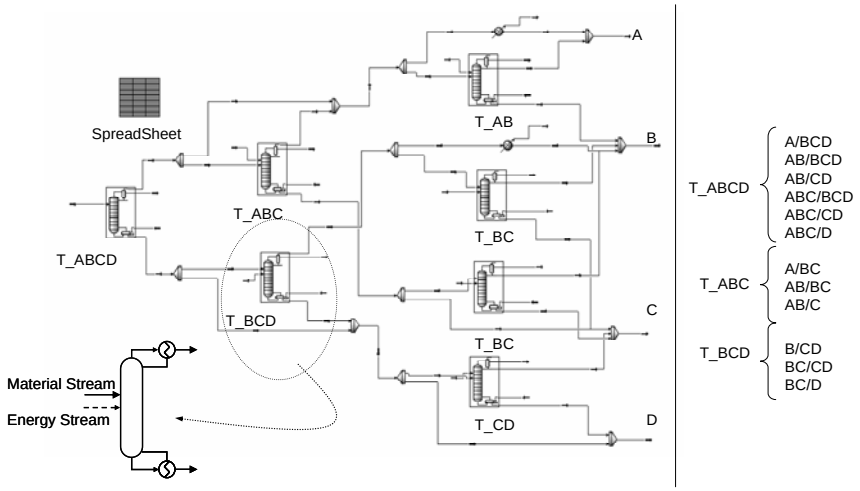

Figure 2. Implementation in HYSYS of a superstructure for a mixture of 4 components. The Energy flows are controled through the spreadsheet. The particular separation in each column

Therefore, the problem is solved using a logic based decomposition algorithm that takes advantage of the structure of the problem iterating between those levels.

2.2. Inner optimization level. Fixed sequence of columns.

In this level we have fixed the sequence of columns. This problem is by itself a non-linear disjunctive problem in which we simultaneously optimize the operational parameters, the number of trays and the feed tray position. An algorithm for solving this problem using process simulators was proposed by Caballero et al [4]. In this approach each column is defined with a number of trays large enough to include the optimal solution. Distillation trays are classified in existing or non-existing trays (non-existing trays behave like simple bypasses without mass or heat exchange). The algorithm starts by solving an initial NLP problem for a fixed number of trays. (i.e. initially all trays exist). From the solution of this NLP a Master problem is defined. This Master problem is formed by two contributions: a) linearizations of the objective function and constraints –like in the outer approximation algorithm for solving MINLP problems- and a contribution that measures what is the change in the objective function and constraints with respect the optimal NLP solution, when new trays are added or deleted. Further details can be found in [4]. Instead of applying the algorithm to each column, that could be very time consuming all columns for a given sequence are optimize simultaneously. The solution of the inner problem is a possible solution to the problem and then a valid upper bound.

2.3. Outer Optimization level: Structural level.

To select a new configuration to test in the inner level we solve a Master formed by linearizations of the objective function and constraints of the optimal solution in the inner problem. However, in order to get a valid approximation of the problem it is necessary to take into account two important considerations: a) We must obtain a sub-set of initial solutions that include all the separation tasks of all the columns. Note that, although a given column can perform different separations, from a mathematical point of view they are different columns. b) Heat exchangers in the superstructure must be assigned to actual columns. Here it is important to take into account that in the superstructure the heat exchangers are separated from the columns, i.e. condenser producing A can be assigned to columns A/BCD, A/BC or A/B depending on the sequence. Turkay and Grossmann [4] proposed to solve a set covering problem to select the minimum number of sequences, but in this case the number of possible separations in first column is also the minimum number of problems to be solved. i.e. six for a four component mixture, or 10 for a mixture of five components.

3. Example

Let us illustrate the methodology with the separation of a mixture of four hydrocarbons (C6-C9). The objective is to obtain each one of the components with a purity higher than 95% (in moles) at minimum cost. Initially all the columns were defined with 40 trays, with the feed tray placed in tray number 20 (up-down numbering). In each section 5 trays were defined as permanent (always exist) and the rest were conditional trays. Initially it is necessary to solve six sequences that include all the separation tasks. Figure 1 shows these sequences. The solution of each one of these initial problems include a complete description of the system including the optimal operation conditions number of trays in each section, composition flows etc.

HYSYS.Plant© was used as the simulation tool. Through its COM communication capability a link was established with Matlab©. All the process is controlled from Matlab that contain the disjunctive formulation and include the decomposition algorithm. NLP subproblems were solved using SNOPT, and LP, MILP problems were solved using CPLEX through the MATLAB-TOMLAB gate link.

When all the separation sections have been initialized Master MILP problem is generated by the linearizations of the objective function and the external constraints – in this case purity specifications-. This master includes logical relationships in order to assure structurally feasible solutions and binary cuts to prevent repeated solutions. The solution of the outer Master problem predicts a new sequence of columns that is optimized in the inner level. The procedure is repeated until the outer Master produce an objective higher than the best problem in the inner level and the new sequences (all except those used in the

initialization) do not produce improvement in the objective function. This double stopping criteria is used to minimize the probability of get trapped in local solutions due to the non convex nature of the problem.

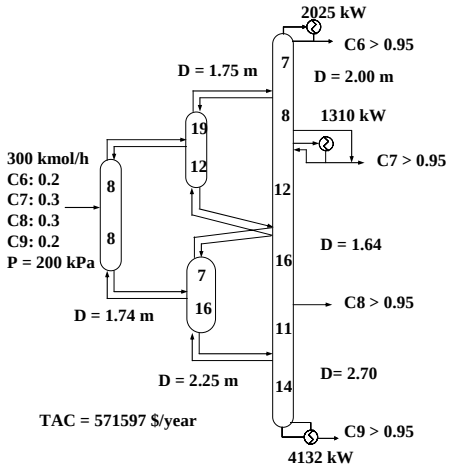

Figure 3. Optimal solution in example. Numbers in each column section are the number of trays. Table in the right side shows the partial results obtained by the proposed solution algorithm.

Column Sequence (Initial sequences)	**TAC** ($/year·$10^4$)
ABC/BCD; AB/BC; BC/CD; A/B; B/C ;C/D	**57.16**
AB/CD; A/B; C/D	66.68
AB/BCD; A/B; B/CD C/D	66.04
A/BCD; BC/D; B/C	74.46
ABC/CD; A/BC; B/C; C/D	63.81
ABC/D; AB/C; A/B	68.51
1. Outer Master	*37.25*
1: ABC/D; A/BC;B/C	78.62
2. Outer Master	*50.21*
2. A/BCD; BC/CD; BC	62.97
3. Outer Master	*52.78*
3. A/BCD; B/CD; C/D	66.02
4. Outer Master	*58.73*
ABC/BCD; A/BC; BC/CD; B/C; CD	62.47
5 Outer Master	*61.98*

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