PROSYN - An Automated Topology and Parameter Process Synthesizer

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EDRC 06-139-92

PROSYN - AN AUTOMATED TOPOLOGY AND PARAMETER PROCESS SYNTHESIZER

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ABSTRACT

This paper describes an improved, user friendly version of the computer package PROSYN - a mixed-integer nonlinear programming (MINLP) process synthesizer. PROSYN is an implementation of the modeling and decomposition (M/D) strategy by Kocis and Grossmann (1989) and the outer approximation and equality relaxation algorithm (OA/ER) by Kocis and Grossmann (1987). Main characteristic of the new version of PROSYN is that it enables automated execution of simultaneous topology and parameter optimization of processes. Optimization of each NLP subproblem is performed only on the existing units rather than on the entire superstructure which substantially reduces the size of the NLP subproblems. In order to reduce undesirable effects of nonconvexities involved in the master problem the OA/ER algorithm has been improved by the use of an augmented penalty function. A simple process simulator has been built in to perform automated initialization of the first NLP step. A comprehensive PROSYN's library of models for basic process units and interconnection nodes, and a comprehensive library of basic physical properties for the most common chemical components have been developed. This enables to carry out an automated generation of a complex model representation for a superstructure in which the topology is specified by a concise interface. PROSYN allows to run in interactive mode and thus provides the user with a good control and supervision of calculations instead of having the procedure to be totally automated. PROSYN allows to carry out process synthesis at two basic levels of complexity: MINLP optimization through M/D and simultaneous heat integration Including HEN costs. Applications with PROSYN are demonstrated with two example problems.

KEYWORDS

Heat integration; MINLP; process optimization; process synthesis; PROSYN; synthesizer.

INTRODUCTION

Although substantial progress in flowsheet synthesis has been recorded in the near past, it is clear that current capabilities of mathematical programming have not yet been fully explored in the area. In this article recent development of a new version of MINLP process synthesizer PROSYN is presented. The current user friendly version of PROSYN is a further development of a preliminary prototype package (Kravanja and Grossmann, 1990). It is an implementation of the most advanced optimization techniques for solving process synthesis problems that are formulated as MINLP problems.

Technical Background

The initial NLP subproblem can be significantly reduced by applying the general M/D scheme that is applied to decompose the initial NLP substructure problem into existing flowsheet to be optimized and other nonexisting units to be suboptimized using a Lagrangean suboptimization procedure to obtain information about nonexisting units. At each NLP subproblem, only the existing units are optimized rather than the entire superstructure without compromising the optimality of the **MINLP** algorithm. All NLP subproblems are thus significantly smaller and many numerical difficulties are thus circumvented.

PROSYN enables simultaneous topology and parameter optimization of the process **using the OA/ER algorithm. The algorithm consists** of **solving** an alternating **sequence of nonlinear programming (NLP) and** mixed-integer linear **programming (MILP) optimization problems. The former corresponds** to the **optimization** of **parameters for a flowsheet with** fixed structural topology and yields an **upper** bound to **the** objective **to be** minimized. The latter **involves** a **global approximation to the superstructure** of alternatives in **which a new topology is identified such that its lower** bound **does not exceed the current best upper bound. The search is terminated when the predicted lower bound exceeds the upper bound. Alternatively, the search can be stopped when there is no improvement in the NLP subproblem. MINOS (Murtagh and Saunders, 1985) is used to solve the NLP subproblems and SCICONIC (SCICON, 1986) is used to solve the MILP** master **problems.**

Presence of nonconvex functions in the models of process units and interconnection nodes may cut off the global optimum. In order to reduce undesirable effects of nonconvexlties involved in the master problem the *OA/ER* algorithm has been improved by the use of penalty function that allows violations of linearizations of nonconvex constraints in the infeasible region and thus makes possible to obtain feasible solution in spite of nonconvexities (see Viswanathan and Grossmann, 1990). Another very important procedure to remove the effect of nonconvexities that has also been implemented into PROSYN, is a linearization modification procedure by Kocis and Grossmann (1989) by which linearizations associated with the part of superstructure not selected in the master problem become redundant. This deactivation of the linearizations establishes the feasibility of the linearizations at zero conditions.

Program description

The flowchart of PROSYN is shown in Fig. 1. The main part of PROSYN are command files and logic that supervise the M/D and OA/ER procedures, and that communicate with GAMS (General Algebraic Modeling System), an interface to NLP and MILP solvers by Brooke et al. (1988). The other part comprises an automated model generator and NLP initializer that uses a simple process simulator. In terms of complexity, the problems can range from a simple NLP optimization problem of a single process unit up to MINLP optimization of a complex superstructure problem with simultaneous heat integration including HEN costs.

The Model Generator. Interface for an automated generation of the superstructure comprises firstly, a specification of a superstructure

topology with a simple configuration data file (Fig.1, p_struct.dat) and secondly, a command procedure that according to a given superstructure topology, automatically generates the complex input model representation of a superstructure out of PROSYN's library. The superstructure of alternative flowsheet structures is represented in terms of interconnection nodes (splitters and mixers) and process unit nodes (reactors, compressors, distillation columns, etc.). Here the process superstructure is modeled in composite form since subproblems at each step of the M/D strategy and the OA/ER algorithm comprise different number of constraints, different objectives and variable space of process variables.

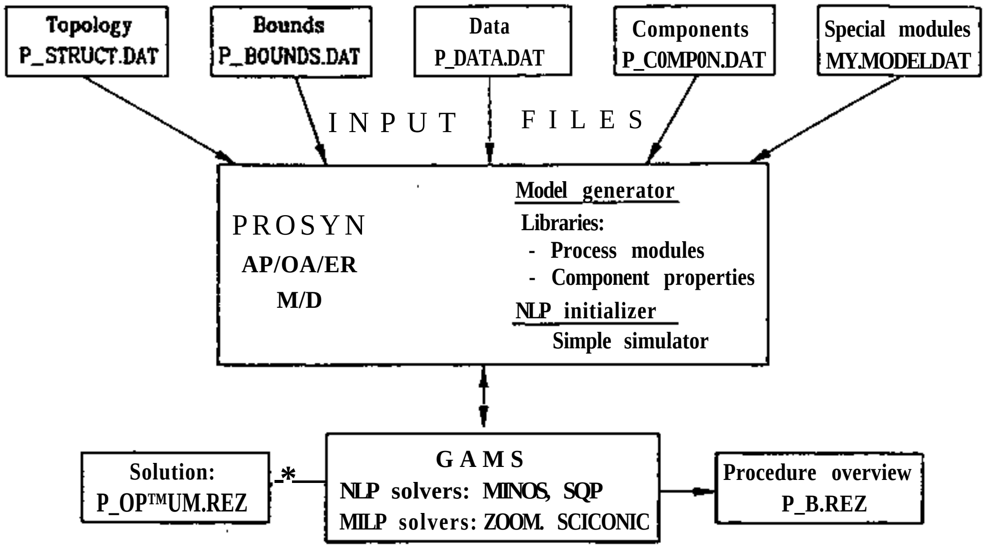


Fig.1. Flowchart of PROSYN.

PROSYN's Library. For each basic process units and interconnection node a module in equation form has been developed and built in PROSYN's library. Also, a library of basic physical properties has been developed that uses data given by Reid at al. (1987), for the most common chemicals. Both libraries can be easily accessed to complete it with models for eventually missing process units and/or interconnection nodes, as well as with missing chemicals or properties. As an interface for mathematical modeling and data inputs, the high level modeling language GAMS is used.

NLP Initializer. It is clear that the quality and efficiency of the NLP subproblems are highly dependent on the starting point supplied. However, to supply a good one is not a straightforward task. In order to facilitate the task, a very simple process simulator that becomes a part of the PROSYN library, has been developed. It uses the same equations as the models for process units and interconnection nodes. All what the user has to supply are some guesses such as compressor outlet pressure, conversion of key component in reactors, etc. The initialization is performed automatically for the first NLP step, while for other NLP subproblems it could be performed when the previous master problem does not provide good starting points for successive NLP subproblems that fail to converge. Our experience has shown significant computational time savings of the NLP optimizations using this approach.

Execution of PROSYN

PROSYN provides the user with a good control and supervision of the calculations instead of having the procedure to be totally automated. Although PROSYN can run in automated mode, the interactive mode is very useful when dealing with a complex problem which could cause the optimization to fail if PROSYN ran in automated mode. The user has to provide five input data files: definition of topology, upper and lower bounds of process variables, data like utility and investment costs, a list of chemical components, and if necessary,special model equations and an initialization scheme that are not present in PROSYN's library.

EXAMPLES

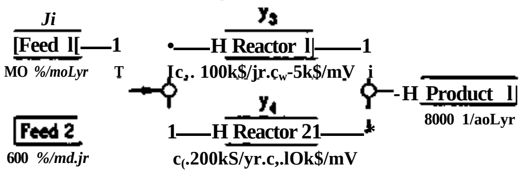
The applications with **PROSYN** will be demonstrated with two examples of increasing complexity. **The** first small example will illustrate steps of the **optimization procedure using M/D strategy. The second** example **will illustrate synthesis of a medium-size process by simultaneous heat integration including HEN** costs.

Example 1

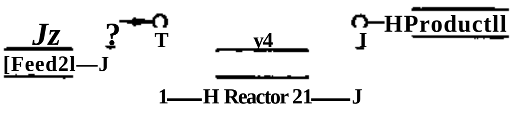
The superstructure of the Example 1 (Fig.2a) comprises two alternative raw material feeds with different costs and concentrations of reactants, and two alternative catalytic reactors with different efficiencies and investment costs. The objective of the problem is to identify an optimal trade-off between raw material costs and investment costs for the mentioned alternative cases. The problem has been formulated as an MINLP problem with four different topologies embedded in the superstructure. Existence binary variables Yl and Y2 have been assigned to the feeds, and Y3 and Y4 to the reactors.

I. First NLP and Decomposition.

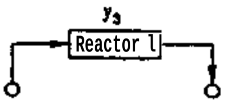
The superstructure has been decomposed into two structures - one initial flowsheet and one subsystem of nonexisting unit. Optimization of the initial flowsheet (Fig.2b) has been carried out for topology y= (0,1,0,1). It should be noted that PROSYN automatically activates only that part of model which is related to existing units (y2=l - feed 2, y4=l - reactor 2). Since direction of the optimization is maximization of revenue, the solution of 1,068,900 $/yr gives the lower bound to the objective. The next step is derivation of linear approximations to the nonlinear equations of reactor 2 and modification of linearizations for zero conditions. PROSYN derives also an integer cut constraint that prevents the MILP master problem to repeat the topology.



a) Superstructure



b) Initial flowsheet



c) Subsystem

Fig.2. Superstructure, initial flow-sheet and subsystem of Example 1.

Suboptimization of subsystem (Fig.2c) has been performed for topology y =

(0,0,1,0). In order to supply to the MILP master problem a linear approximation of nonexisting units, only nonexisting units that are represented by nonlinear model, have to be suboptimized. Since feed 1 is represented by linear relations only, it is therefore excluded from the subsystem. Input variables of reactor 1 are automatically fixed to the optimal condition of rector 2 that has been found at the optimization of the initial flowsheet. In the objective, the Lagrange multipliers for the splitter component balances obtained at the optimization of the initial flowsheet, are supplied as inlet material costs while the multipliers for the mixer are supplied as outlet product prices. The solution yields revenue of 375,900 $/yr. The next step is again the derivation of a linear approximation, now for reactor 1.

II. First MILP Master Problem. Both linear approximations together with all the linear equations originally embedded in superstructure model, represent the global linear approximation of the whole superstructure. The solution of 1,168,000 $/yr yields the upper bound to the objective and predicts the new topology y=(0,1,1,0).

III. Second NLP Subproblem. According to the given topology predicted by the master problem, PROSYN constructs for the NLP stage 2 a nonlinear model for existing feed 2 and reactor 1 while nonexisting units are temporarily excluded. Since the solution is 746,000 $/yr the procedure is terminated. The optimal solution is the one found in the first NLP subproblem for topology y=(0,1,0,1).

Example 2

In the second example, the simultaneous approach has been extended also for HEN costs using simultaneous model for HEN by Yee et al. (1990a) and Yee and Grossmann (1990). The model can simultaneously target for both area and energy costs at variable temperature driving forces of matches and stream arrangement for non-uniform stream film coefficients. Moreover, it does not rely on the pinch point concept by which an original network has to be partitioned into subnetworks. It also enables easily to handle constraints on the matches. The model was formulated either as the NLP targeting problem for area and energy or as the MINLP problem for HEN synthesis. There are two drawbacks of the NLP model: the fixed costs cannot be accounted for the HEN and the mathematical expressions for the area costs of the matches are highly nonlinear and nonconvex. On the other hand, the main drawback of the MINLP model is that it introduces significant number of binary variables. Since in MINLP optimization of the process flowsheets the main bottleneck in terms of complexity and consumption of CPU time usually lies in solving NLP subproblems, the NLP model for HEN at the first glance appears to be more favorable than the MINLP one. However, the high nonlinearities and nonconvexities in the NLP model for HEN can seriously reduce the efficiency of the OA/ER algorithm. That is why only the MINLP version of HEN model has been successfully applied for the simultaneous MINLP optimization of the process and its HEN, while the use of the NLP model for HEN has been restricted only to fixed topology of the process flowsheet (Yee at al, 1990b).

In order to perform the simultaneous MINLP optimization approach using the M/D strategy, a new NLP version of HEN has been developed. A special logic involved in the model, takes care that according to the M/D strategy at each NLP subproblem only existing process streams and utilities are taken in the optimization, while nonexisting ones are temporarily excluded without compromising the optimality of the MINLP problem. Although the new version of the nonlinear HEN model is more robust than the original one,

and although the OA/ER algorithm in PROSYN has been improved by the use of the penalty function to reduce undesirable effects of nonconvexities, the troublesome impacts of the highly nonconvex HEN model are usually so strong that the original master problem of the OA/ER algorithm fails to predict a good starting point for the next NLP stage. Moreover, the values of process variables are usually shifted either to their upper or the lower bounds which prevent the next NLP subproblem to converge to its feasible solution.

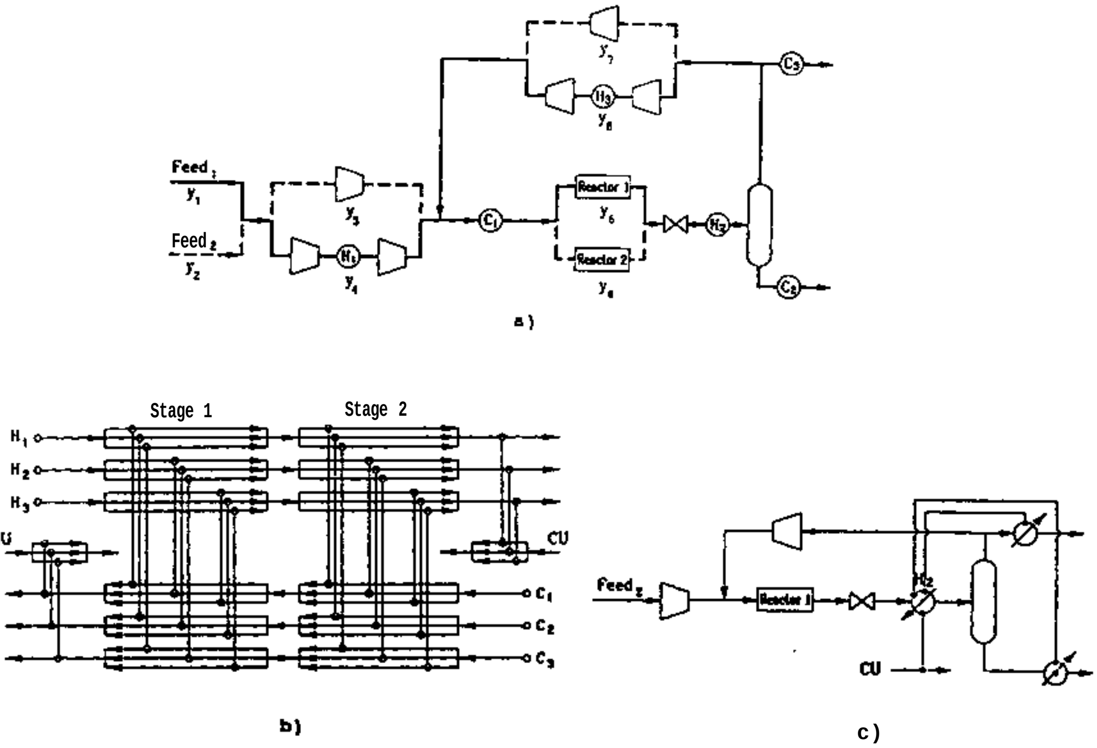


Fig.3. Example 2: a) Superstructure and initial flowsheet (bold line), b) HEN Superstructure for initial flowsheet, c) final flowsheet.

In order to further improve the efficiency of the simultaneous procedure by the PROSYN, two optimization scheme has been proposed. By the former (a), after each master problem an initialization of the next NLP stage is performed by the use of the simple simulator, while by the latter (b), the linear approximation of the highly nonconvex area costs terms is developed only once and consequently, less nonconvexities are introduced into the [illegible] Both schemes has bam tested on [illegible] example previously described and investigated by Kravanja and Grossmann (1990). The superstructure of the process (Fig.3a) includes 16 alternative flowsheets and the superstructure of Its HEN (Fig.3b) about 16.7 million alternative networks. The objective of the problem is to find an optimal heat integrated process flowsheet that yields maximum revenue. Results of the OA/ER algorithm for both optimization schemes are given in Table 1. Due to [illegible] of nonconvexities in both cases the master problems have [illegible] a valid upper bound to the objective to [illegible] maximize [illegible] procedures have been applied until no improved [illegible] found [illegible] the use of [illegible] schemes [illegible] same optimal flowsheet (Fig. 3c) has been found and both solutions yield the same revenue of 2,613.000 «/yr. The revenue is 768,000 «/yr higher than the [illegible] fixed [illegible] topology by [illegible] at al. (1990b) [illegible] 2.9oto00 [illegible] higher than the one obtained by Yee at al. (1990b) using heat integration model by Duran and Grossmann (1986). Although the optimal topology [illegible]

to be the same as the fixed one studied by Yee at al. (1990b), the revenue is much higher due to more efficient handling of nonconvexities. Since nonconvexities in the case a) are accumulated through the OA/ER procedure, they cut off more of the feasible region of the master problems than the nonaccumulated ones in the case b). Consequently, the results of the master problems in the case a) decrease more rapidly by the number of the OA/ER iteration when compared to the case b). Also, no initializations for NLPs in the case b) but for the first one are needed. This clearly indicates that scheme b) for simultaneous optimization of the process flowsheet and HEN is more robust than the scheme a).

Table 1. Results for Example 2.

Iteration	Topology y	NLP (CPU time) k$/yr	MILP (CPU time) (sec on MicroVax 3100)
	MINLP optimization scheme a)		
1	(1,0,0,1,1,0,0,1)	2240 (101)	2173 (89)
2	(0,1,1,0,1,0,1,0)	2613 (59)	606 (95)
3	(1,0,1,0,0,1,0,1)	1818 (113)	and terminated
	MINLP optimization scheme b)		
1	(1,0,0,1,1,0,0,1)	2240 **(101)**	2173 (89)
2	**(0,1,1,0,1,0,1,0)**	2613 **(41)**	**1943** (122)
3	**(0,1,1,0,1,0,0,1)**	2563 **(106)**	**and terminated**

CONCLUSIONS AND SIGNIFICANCE

The first prototype version of PROSYN had the important drawback that the user was required to provide a complex model representation for the superstructure and complex logic relations of the M/D strategy. In the new version of PROSYN the logic has been automated, a library of models for process units and interconnection nodes has been built in, and data of basic physical properties has been added which has made PROSYN much more user-friendly. In this way all user's input files are now very simple and concise. Another very important improvement concerns the *OA/ER* algorithm. In order to handle nonconvexities the algorithm has been modified by adding augmented penalties in the master problem. Further development of PROSYN has been done by introducing a simple simulator that initializes the first NLP step. With the aid of the new capabilities, PROSYN enables to carry out automated MINLP topology and parameter optimization of complex process superstructures. PROSYN is an attempt to develop an advanced tool for process design that can handle real, large scale and complex engineering problems. It can be of high significance especially in decision making of design engineers when exploring large number of alternatives.

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