Multilevel-hierarchical MNLP Synthesis of Process Flowsheets

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Abstract The objective of this contribution is to propose a multilevel-hierarchical approach to the MINLP synthesis of process flowsheets. Following a hierarchical strategy, the designer can postulate the superstructure at different levels of representation of flowsheet alternatives and model it at the corresponding level of aggregation and complexity. By the use of the prcscrcening procedure the superstructure is optimized more effectively and reliably. The approach enables one to address different process operations like reactions, connectivity and species allocation, separation, energy and heat integration and HEN through simultaneous superstructure optimization.

INTRODUCTION

Process flowsheet synthesis concepts are based either on heuristic generation, evolutionary modification, tasks targeting or superstructure optimization. While the former two concepts are driven purely by designer experience and creativity throughout the synthesis, the latter ones are based on mathematical programming which leaves the designer to creatively propose targets and superstructure of flowsheet alternatives, and formulate adequate aggregation/disaggregation of MINLP superstructure models. The solution of these concepts mainly depends on the availability and the quality of supplied information used to construct targets and superstructures. The advantage of the task targeting optimization concept over the superstructure optimization concept is that it enables to simultaneously consider different phenomena from the overall process performance viewpoint. On the other hand, the superstructure based concept involves task integration, and hence, the flowsheet topology is represented in a more natural and straightforward way. As for the solution of the MINLP, the size of the NLP problems can be significantly reduced by the use of the Modelling and Decomposition strategy (Kocis and Grossmann, 1989) by performing NLPs only for the existing flowsheet rather for the whole superstructure which is very difficult and expensive to solve. However, one of the main problems with the superstructure approach is that it is still limited to problems of medium size and complexity due to the limited capability of the current MINLP optimization algorithms. Consequently, many good alternatives can be left out of the superstructure solution space. Hence, there is an incentive to propose a more general framework for the process synthesis which can efficiently overcome the drawbacks of the superstructure approach.

Thus, the main objective of this paper is to propose a framework by which it is possible to postulate, prescreen and optimize the superstructures in a more systematic manner, and to show on an illustrative process example the advantages of using the superstructure approach.

MULTILEVEL MINLP APPROACH

A multilevel-hierarchical MINLP framework for the synthesis of process schemes is proposed. Its main features are as follows:

- It follows the hierarchical strategy of process synthesis (Douglas, 1988, Siirola, 1996) from reaction path (species identification) to plant connection (species allocation) to phase separation and energy and heat integration.
- It is a thorough combination of hierarchical strategy of process synthesis and MINLP superstructure approach. It starts with reactor network synthesis (MINLP1), proceeds with separation synthesis (MINLP2) and finishes with heat exchanger network synthesis (MINLP3).
- As opposed to the multilevel strategy by Daichendt and Grossmann (1994, 1997) thermodynamic models are not used at the higher levels, but instead simplified models.
- It can combine the different synthesis concepts so as to hierarchically examine different tasks regarding their identification, targeting and integration.
- The Modelling and Decomposition strategy is utilized in order to handle complex and large-size superstructures.

Following the hierarchical strategy, the superstructure is postulated at different abstract representations of flowsheet alternatives, which are modelled at different levels of aggregation and complexity. The more the synthesis is concerned with task targeting, the more the models are aggregated and made simpler. On the other extreme, at lower levels the superstructure represents the full space of flowsheet alternatives. Here the unit and interconnection node models are more detailed. Since the aggregated models underestimate the original models, their optimization provides a rigorous upper bound to the profit to be maximized. This makes possible the bounding procedure to rigorously eliminate poor suboptimal alternatives.

Algorithmic approach to the multilevel MINLP approach

Since the most general algorithm for N level MINLPs is rather complex, the one for two-level approach is outlined here as follows:

Step 1: Solve MINLPl to obtain an upper bound on the profit and binary variables for substructure selection (could be individual units or groups of units like entire distillation train or not).

Step 2: For fixed binary variables solve MINLP2. This could be NLP if individual units are chosen by binary variables, or MINLP if it is a group of units. The solution gives lower bound.

Step 3: Add an integer cut and perhaps some other bounding information (e.g. Profit ^ Lower Bound) and resolve MINLPl. Continue iterating until bounds are within specified tolerance.

For each additional level the algorithm would have an additional iteration loop within which all higher level iteration loops have to be sequentially converged before one would proceed to an lower level MINLP. Although the algorithm is rigorous, it may need many iterations, especially when the synthesis is hierarchically decomposed to three or more levels. Another problem with this scheme is that simplified models in higher MINLP levels give poor bounds (too overestimated) so that the bounding property cannot be exploited unless tighter constraints are supplied to the MINLP which is not a straightforward task. Rather than iterate all inner loops, a simplified scheme is proposed for 3 levels MINLPs:

<u>MINLPfLevel=l^: Reactor network synthesis,</u>
identification of separation and other auxiliary operation (detailed reactor network model, simple separation model to identify separation tasks, Duran's model to target heat integration)

-> UPPER BOUND PROFIT

<u>MINLPfLevels2V Separation and reactor network</u> synthesis based on identified separation in MINLPl (detailed reactor and separator models, Duran's heat integration)

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<u>MINLPfLevels3): HEN synthesis</u>
at fixed reactor and separation structure (detailed reactor and separator models, modified Yee's MINLP model for heat integrated HEN synthesis)

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-> iterate with MINLP2

As can be seen, the iteration loop between MINLPl and MINLP2 is avoided which considerably reduces the computational effort The superstructure is evolved based on selection of integer variables. In MINLPl the superstructure is developed fully only for the reactor network, whilst for the separation it only uses alternatives with simple models to identify separation tasks. In MINLP2 the superstructure is then expanded for the separation trains or subgroup of units for selected integer variables while the rest of simplified alternatives remain to account properly for reactor-separation interaction. It should be noted that Duran and Grossmann (1986) model for simultaneous heat integration is used at both steps. It identifies hot and cold streams for HEN synthesis. In MINLP3 the superstructure is reduced for reaction and separation to the optimal structure selected at MINLP2, and expanded for HEN synthesis using MINLP model for simultaneous HEN synthesis (Yee and Grossmann, 1990).

Thus, the multilevel MINLP framework is conceptually proposed in such a way that the synthesis is performed hierarchically from task identification to task targeting and to task integration. In MINLPl we start with reactor integration, separation identification and identification of hot and cold process streams by targeting for heat integration. In MINLP2 we proceed with separation and reactor integration while process streams are still handled at the level of identification. Finally, in MINLP3 the task integration is fulfilled by simultaneous HEN synthesis and the optimization of the process scheme until bounds between MINLP2 and MINLP3 are closed. During the iterations, in MINLP2 the identification of process streams are combined with HEN costs targeting in order to improve the upper bound.

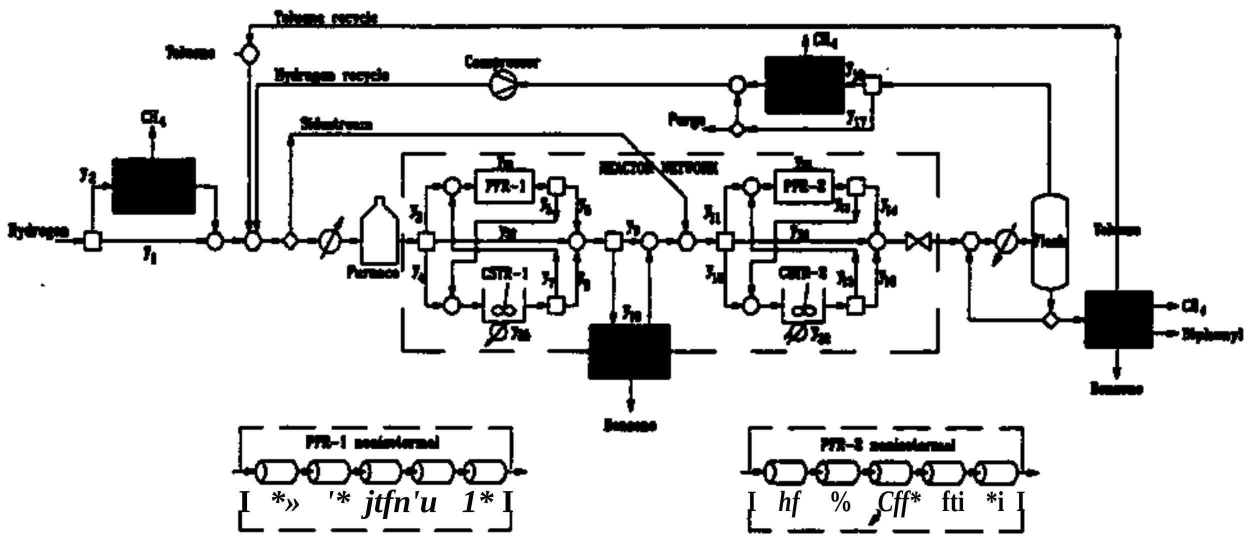
The proposed approach has been implemented in the process synthesizer PROSYN-MINLP (Kravanja and Grossmann, 1994) and is illustrated with an example problem.

EXAMPLE PROBLEM

The HDA process as described by (Douglas, 1988, Kocis and Grossmann, 1989) has been considered as an example problem. The superstructure has been extended for detailed reactor network superstructure, the compact superstructure for the simultaneous synthesis of the multicomponent separation sequence (Novak et aL, 1996) and a proposed one-stage superstructure for HEN. The main objective is to maximize the profit The MINLP synthesis has been performed using the proposed multilevel MINLP framework in just four steps: MINLP1 (reactor synthesis), MINLP2 (separation synthesis), MINLP3 (HEN synthesis) and MINLP2 again to check the bounds.

Reactor network synthesis - MINLP1

The superstructure for MINLP1 is shown in Fig.l. It consists of detailed reactor network superstructure and simplified alternatives for feed and recycle purification and separation. The reactor network comprises two sets of non-isothermal PFR reactors coupled with CSTRs, a side stream and outlet to the intermediate separation in order to decrease the production of a by-product diphcnyl. In each pair of reactors a PFR or CSTR or PFR and CSTR or CSTR and PFR or none can be selected. Each PFR is further composed of five finite elements (small PFRs). An orthogonal collocation on finite elements has been used to discretize and approximate differential equations. MILP step of MINLP1 is used to select the optimal finite element (small PRF) and NLP for optimal reactor outlet condition which are modeled continuously by the parallel Lagrange polynomials (Pahor and Kravanja, 199S). Inlet and outlet temperatures of each finite elements are considered as optimization variables which enable to model PFRs as non-isothermal. The solution gives an optimal temperature profile along each finite element If cooling requirement is zero, it means that the reactor is adiabatic; if it is equal to the reaction enthalpy released, then the reactor is isothermal.



LEGEND FOR INTERCONNECTION NODES
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Fig. 1: Initial reactor network and simplified separation superstructure (MINLP1).

The optimal structure of the initial superstructure problem MINLP1 is shown in Fig.2. The modelling/decomposition scheme has been applied with the optimization of two initial flowsheets (one with PFR-1, another with PFR-2) and with three suboptimizations (CSTR-1, CSTR-2 and recycle purification). Two successive PFRs are selected, the first with four and the second with two segments. The first one turned to be isothermal while the other has outlet temperature less than the inlet one. The solution suggests purification of recycle, no intermediate separation and no feed purification. It yields 6.605 M$/yr which represent the highest upper bound. The solution was found in the 8th iteration using 38 min of CPU time on IBM RISC 6000 43P machine. The size of the problem formulation for the optimal NLP was about 868 equations and 930 variables, and for MILP 1158 equations (873 linearizations) and 5894 of variables (34 binary variables).

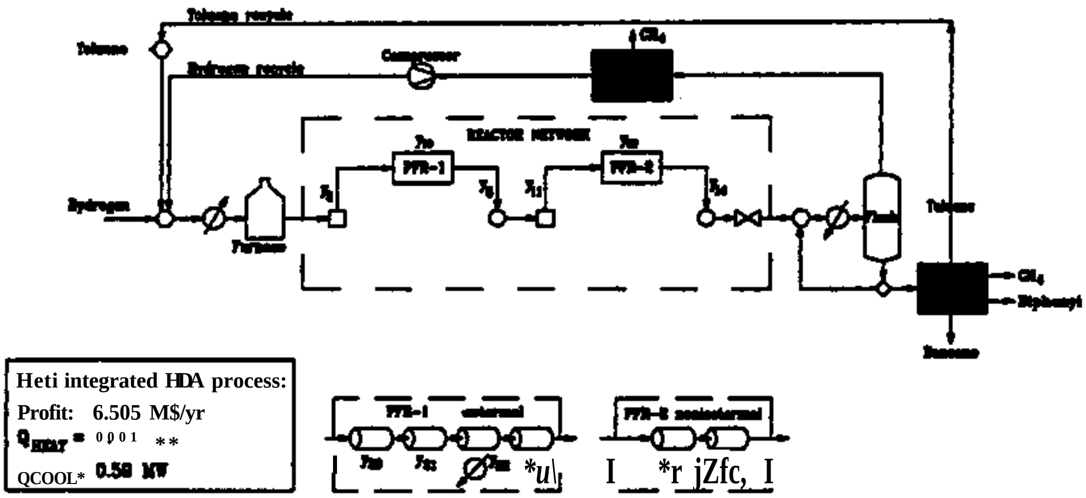

Fig. 2: Optimal structure for initial superstructure problem (MINLPl).

Separation synthesis - MINLP2

Next the superstructure (Fig.3) is expanded for final separation and purification of recycle. A membrane separator with bypass has been chosen for the recycle separation and the compact superstructure for four component distillation sequence synthesis. The main idea of the compact superstructure is to select the path between the columns rather that columns themselves. In this way only three columns were needed compared to ten in the network distillation superstructure. Six binary variables are introduced for the path selection. In addition, either stabilizing column or flash and either diphenyl column or another flash separator can be selected (another four binary variables). Feed purification and intermediate separation remain in the superstructure, but their substructures were not expanded in detail since they were not selected in MINLPl.

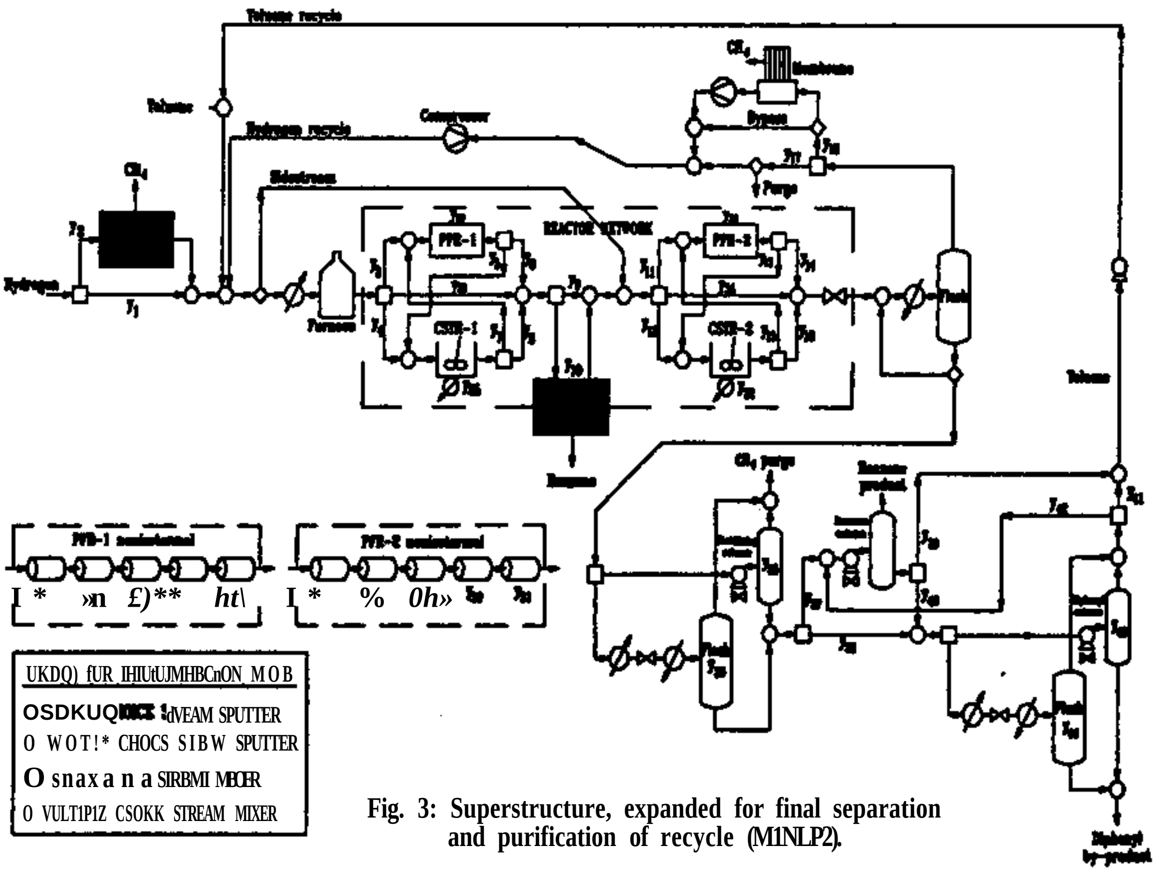

Fig. 3: Superstructure, expanded for final separation and purification of recycle (MINLP2).

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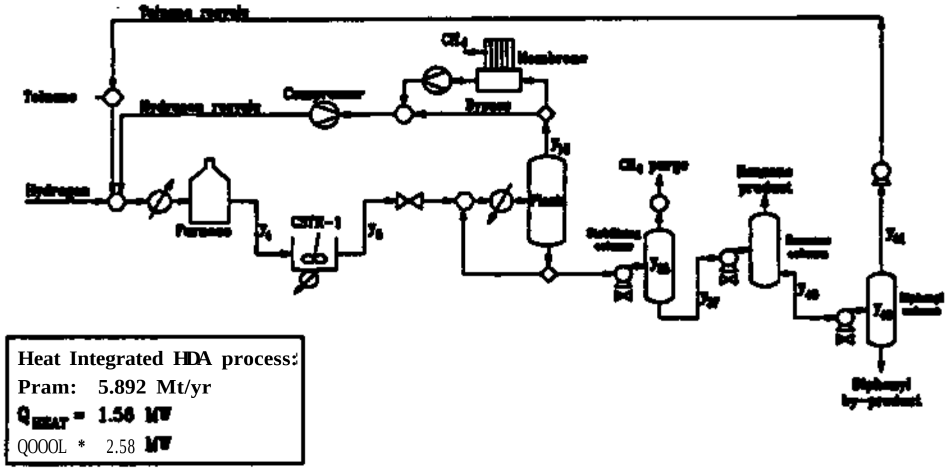

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A superstructure for HEN (Fig.5) has been proposed as an extension of the one by Yee and Grossmann (1990). Since many process streams are isothermal, a one-stage superstructure has been proposed. For isotherms streams it is ideal since just one stage is needed to perform enthalpy balances. In order to fit other non-isothermal streams into the one-stage superstructure, the nonisothermal streams were cut into segments as shown in Fig.5. The resulting superstructure is much more compact and its model is more linear. Additional logic was included to decrease the feasible space further and to make the MINLP optimization approach more robust. Nevertheless, the number of binary variables is still significant: for 10 hot and 7 cold streams and three segments for each non-isothermal stream an additional 151 binary variables were needed.

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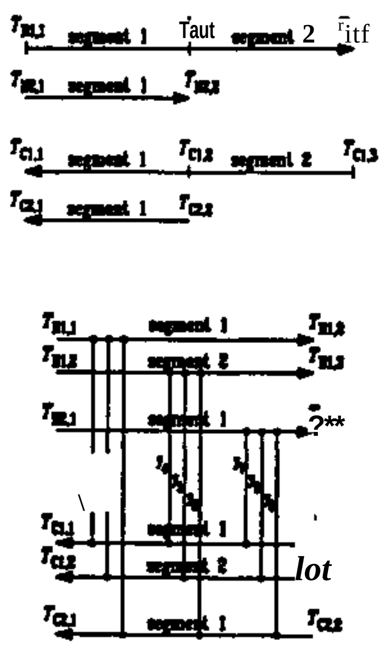

Fig.5: One-stage superstructure for 2 segment hot stream HI, one segment H2, 2 segment cold stream Cl and one segment C2.

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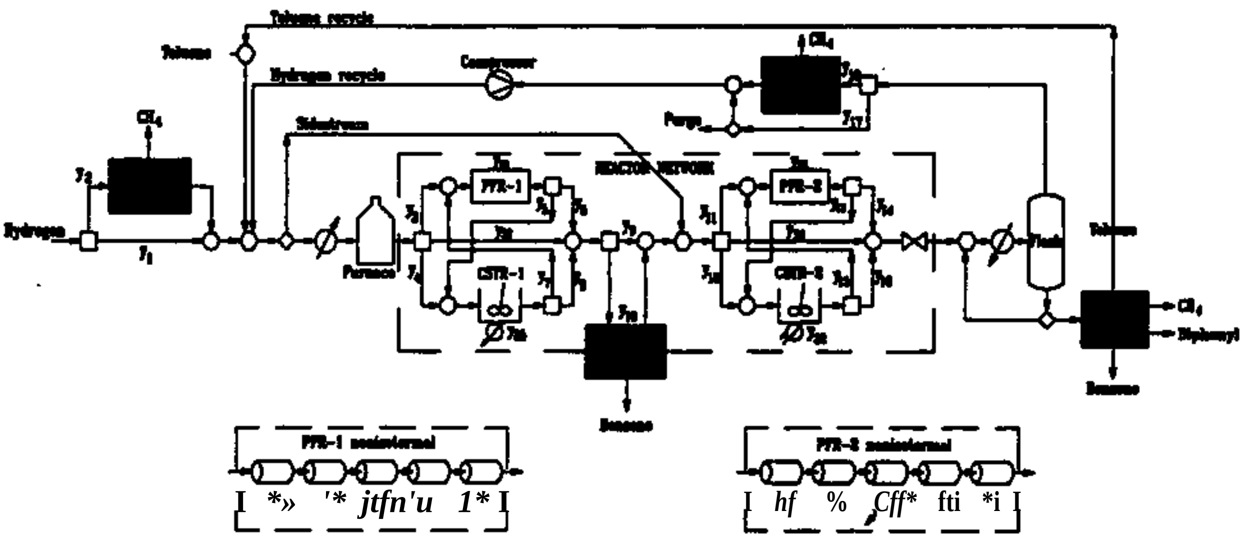
The superstructure for MINLP1 is shown in Fig.l. It consists of detailed reactor network superstructure and simplified alternatives for feed and recycle purification and separation. The reactor network comprises two sets of non-isothermal PFR reactors coupled with CSTRs, a side stream and outlet to the intermediate separation in order to decrease the production of a by-product diphcnyl. In each pair of reactors a PFR or CSTR or PFR and CSTR or CSTR and PFR or none can be selected. Each PFR is further composed of five finite elements (small PFRs). An orthogonal collocation on finite elements has been used to discretize and approximate differential equations. MILP step of MINLP1 is used to select the optimal finite element (small PRF) and NLP for optimal reactor outlet condition which are modeled continuously by the parallel Lagrange polynomials (Pahor and Kravanja, 199S). Inlet and outlet temperatures of each finite elements are considered as optimization variables which enable to model PFRs as non-isothermal. The solution gives an optimal temperature profile along each finite element If cooling requirement is zero, it means that the reactor is adiabatic; if it is equal to the reaction enthalpy released, then the reactor is isothermal.



LEGEND FOR INTERCONNECTION NODES
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Fig. 1: Initial reactor network and simplified separation superstructure (MINLP1).

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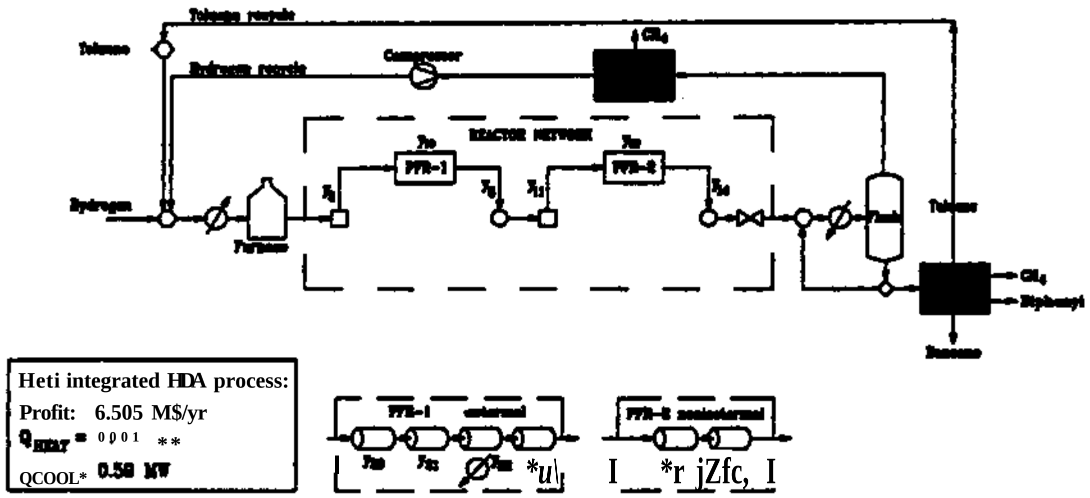

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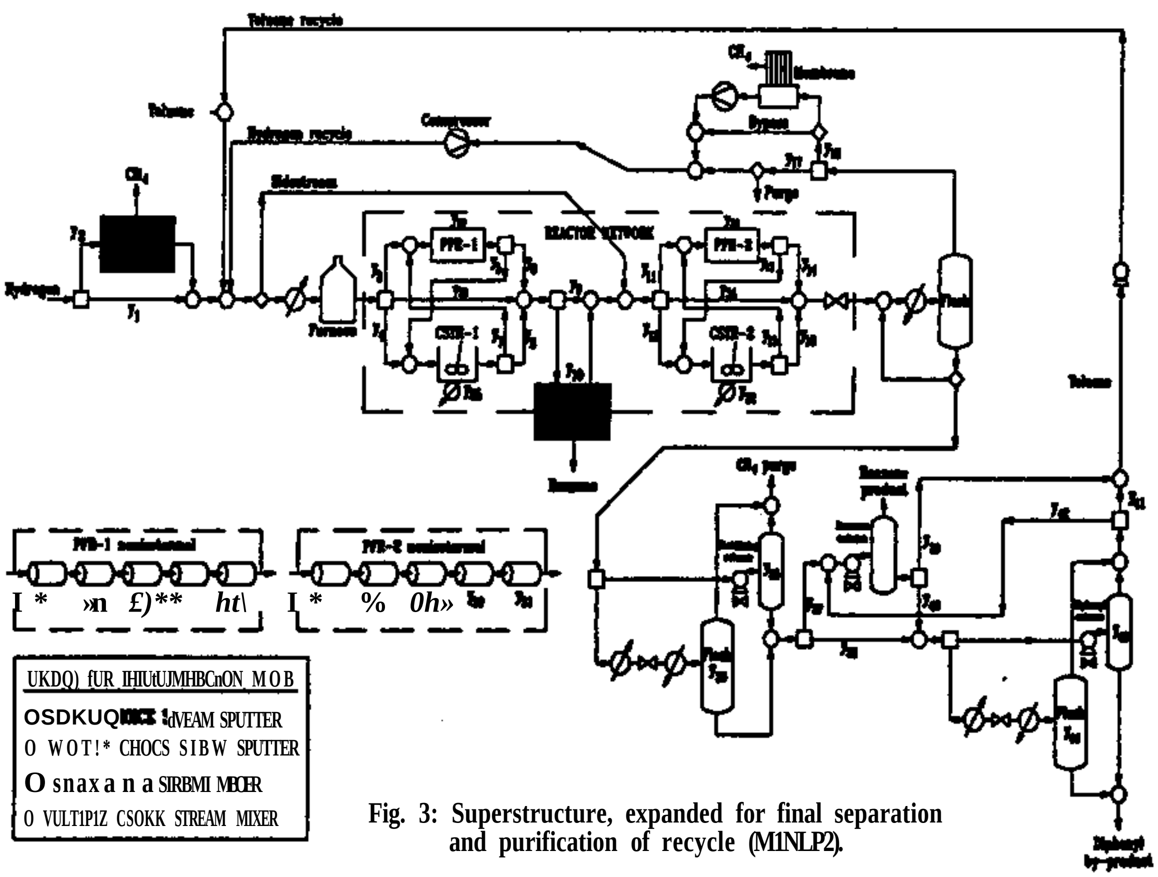

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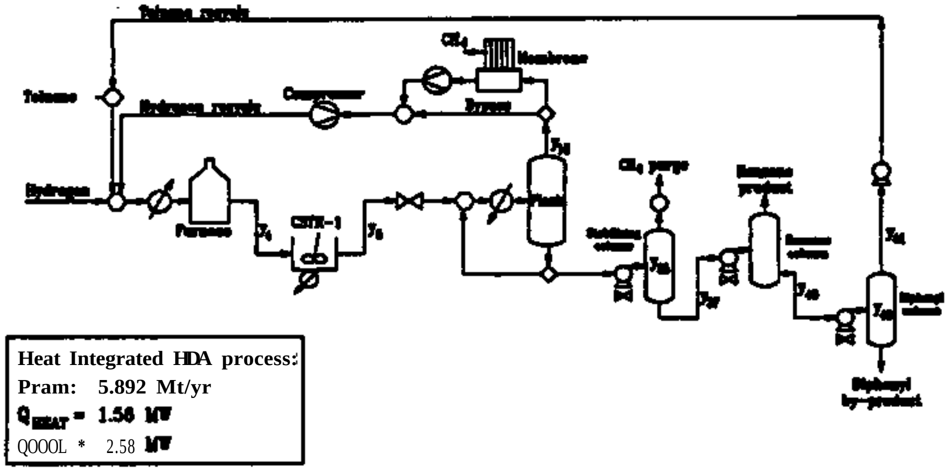

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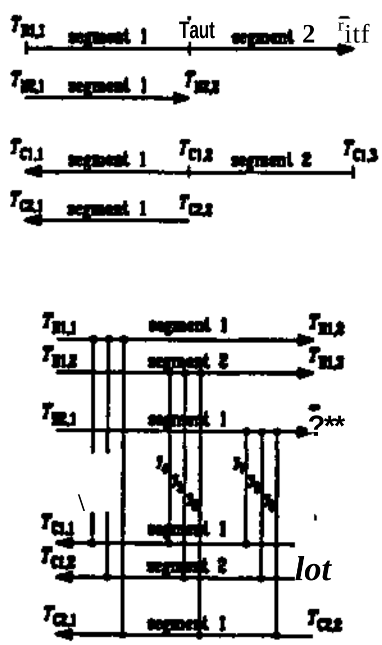

Fig.5: One-stage superstructure for 2 segment hot stream HI, one segment H2, 2 segment cold stream Cl and one segment C2.

Resolved MINLP2

MINLP2 is performed again for the superstructure of Fig.3. Now the Duran's model for heat integration is extended for HEN costs. Very simple cost correlation for the HEN were used. They relate HEN costs to enthalpy exchanged to of from the stream. The optimal solution yields an upper oouna ox 0.24U M^/yr wiin an alternative flowsheet However, since the bounds are very close (5.201 and 5.240), the search is stopped. The final optimal flowsheet is the one on Fig.6. It should be noted that when compared to the solution obtained by Kocis and Grossmann (1989), the flowsheet is now heat integrated and the HEN is synthesized simultaneously.

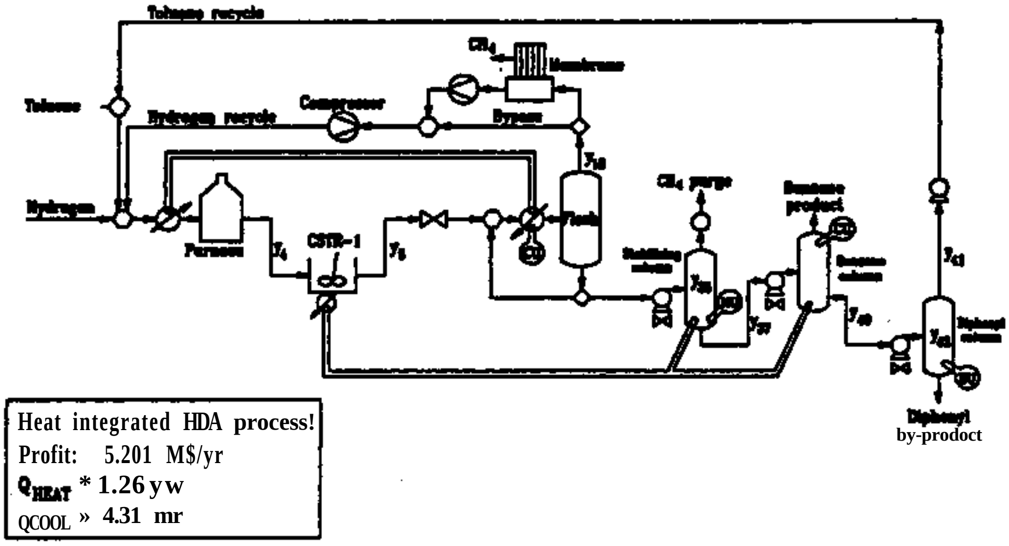

Fig. 6: Optimal nowsheet and its heat integrated HEN (MINLP3).

CONCLUSIONS AND SIGNIFICANCE

The proposed approach is an attempt to improve further the superstructure optimization approach to the synthesis of process flowsheets. The superstructures of process alternatives are generated, prescreened and optimized in a more systematic and reliable way. The approach is also an attempt to combine the hierarchical strategy and the superstructure optimization concept of the process synthesis. This in turn enables the designer to address different phenomena like reactions* connectivity and species allocation, separation, energy and heat integration and HEN synthesis simultaneously in a multilevel MINLP optimization approach.

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