ChE curriculum

DESIGN EDUCATION IN CHEMICAL ENGINEERING

Part 2: Using Design Tools

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THE CONCEPTUAL DESIGN of a chemical process involves the invention of the process, *i.e.*, the selection of the process units, as well as the interconnection between the units. The problem is large, open-ended, and has a very low success rate associated with it. Experienced designers in industry normally complete a conceptual design in two days to a week, look at possible alternatives for another two days to a week, and then use these results to evaluate whether additional design effort can be justified.

In order to teach undergraduate students (with no experience) how to complete a conceptual design, it was necessary to develop several new tools: 1) How to use order-of-magnitude arguments to simplify problems, 2) how to derive design heuristics, and 3) how to decompose very large problems into a set of small, simple problems. With these it is possible to use a very structured approach to inventing petrochemical processes that can be taught to undergraduates. In addition, this systematic procedure can be used as the basis for a hybrid expert system that can complete a conceptual design in one to three hours.

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TABLE 1
Types of Designs

- Order of magnitude estimate *(Error about 40%)*
- Factored estimate *(Error about 25%)*
- Budget authorization estimate *(Error about 12%)*
- Project control estimate *(Error about 6%)*
- Contractor's estimate *(Error about 3%)*

A HIERARCHICAL APPROACH TO PROCESS SYNTHESIS

The tools described in Part I* of this paper are an important part in the evaluation part of flowsheet synthesis. However, we still need to generate these different flowsheet configurations. In order to accomplish this goal we adopt a hierarchical planning procedure, similar to that used by Sacerdotti [1] in ABSTRIPS.

With Sacerdotti's approach, we break the problem down into a hierarchy of abstraction spaces where more detail is added to the solution at each level in the hierarchy. Thus, we develop an initial solution that considers both the starting point and the final goal, but not the details of how we achieve that goal. Then, we improve the solution by considering the next most important set of details, and we continue to add layers of detail in this manner until we obtain a complete solution. This is the same approach described in Table 1, except now we will define a hierarchical plan for Level 1 only. A hierarchical approach of this type has also been used by Meade and Conway [2] for the design of VLSI chips.

In order to develop a hierarchical plan we can look at a number of typical solutions and then consider what happens if we systematically remove detail from the solution. If we can find a general framework for stripping away these layers of detail, then we can re-

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*Published in *CEE*, 21 No. 1 (Winter 1988)

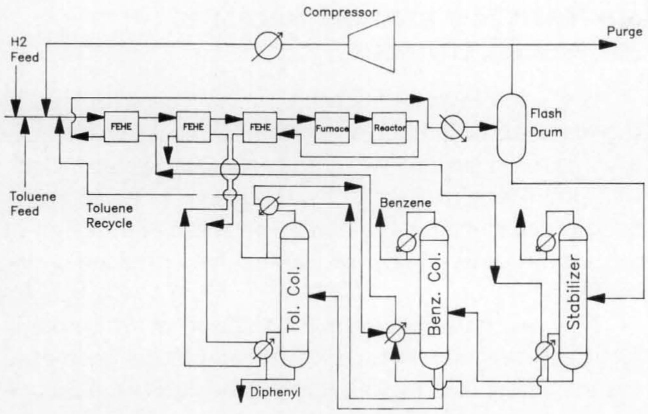

FIGURE 1. HDA process flowsheet (maximum energy recovery)

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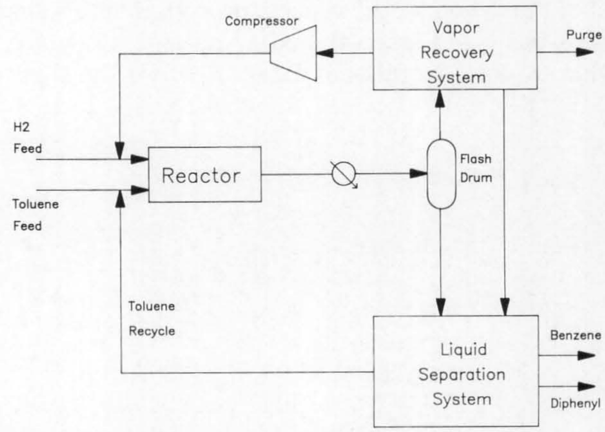

FIGURE 3. HDA process (separation system flowsheet)

verse the order of the levels and obtain the desired hierarchy.

Energy Integration

Suppose we consider an energy integrated flowsheet for the hydrodealkylation of toluene to produce benzene (see Figure 1). If we remove all of the heat exchangers and simply indicate which streams need to be heated or cooled, we obtain the much simpler flowsheet shown in Figure 2. There is a systematic procedure available for designing a large number of heat exchanger network alternatives if we have a flowsheet such as Figure 2.

The particular heat exchanger network that we select normally will affect the optimum values of the process flows, which may affect the best choice of the distillation train. Hence, there may be a weak coupling between the design of the heat exchanger network and the remainder of the process, and we may need to backtrack to our selection of the distillation train in order to find the best solution.

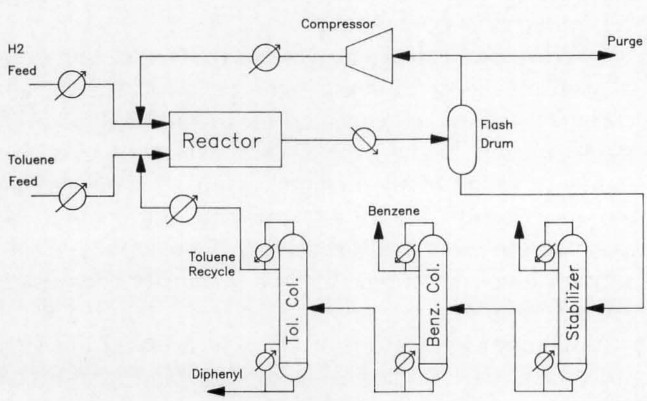

FIGURE 2. HDA process flowsheet

Distillation Column Sequencing

Normally, there are a large number of alternative distillation sequences that can be used to separate a mixture into a series of products. We could use heuristics (see [3]) to decide which alternatives to consider, or we could rapidly generate and evaluate all the possibilities and then consider only those alternatives which are economically feasible. Suppose we remove the distillation train from the flowsheet shown in Figure 2 and replace it with a black-box (see Figure 3). For ideal mixtures, it is always possible to accomplish a set of distillation separations, and the details will have no effect on the equipment remaining in Figure 3. Hence, we strip away the details of the distillation train to simplify the flowsheet.

Vapor Recovery System

Figure 2 does not include a vapor recovery system, but in some cases it may be desirable to include one. There are a number of types of units that we could use as a vapor recovery system (*e.g.*, a gas absorber, a condensation process, an adsorption process), and there are several locations that we could consider and all must be evaluated. If we replace any vapor system in Figure 2 by another black-box unit (see Figure 3), we do not affect the structure of any of the remaining units on the flowsheet and we have further simplified the structure.

General Structure of the Separation System

Not all processes include both a vapor and a liquid recovery system. For vapor-liquid process, there are only three types of situations that can arise, depending on the phase of the reactor effluent (*i.e.*, all liquid, a two-phase mixture, or all vapor). Suppose we lump all of the details of the separation system into a single black-box (see Figure 4), and we specify the details of what to put into this box later. Now we see that we

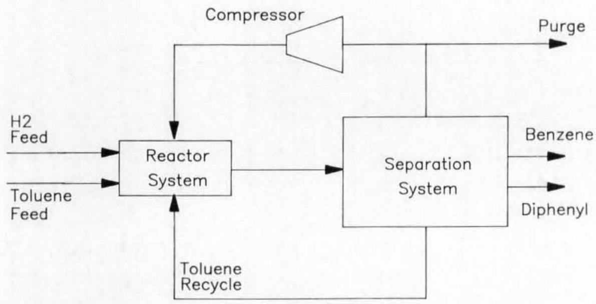

FIGURE 4. HDA process (recycle structure flowsheet)

have stripped away another level of detail, but we still preserve the recycle structure of the flowsheet.

Overall Picture of the Process

Removing layers of detail from the flowsheet has led to significant simplifications, but now suppose we draw a black-box around the complete process. We will be left with the input and output streams (Figure 5). This picture of the process is still significant, because the raw material costs are usually in the range from 33 to 85% of the total processing costs. We can start to focus on the design variables that affect the product distribution and the optimum process flowrates without having to consider any of the other complicating details. From our earlier discussions we know that the optimum values of the process flows will change as we add additional layers of detail to the process, and therefore we must develop the design as a function of the design variables that affect the process flows.

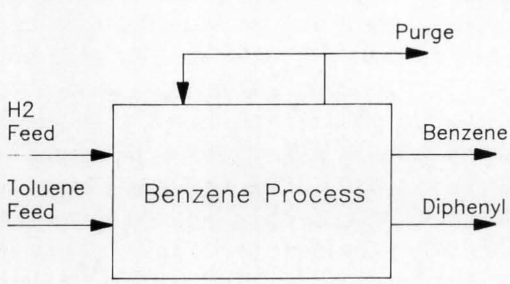

FIGURE 5. HDA process (input-output flowsheet)

A HIERARCHICAL DECISION PROCEDURE FOR PROCESS SYNTHESIS

If we add layers of detail to a conceptual design in the opposite order that we stripped them away in the previous discussion, we obtain the hierarchical decision procedure presented by Douglas [4] (Table 2). (A decision concerning the choice between the design of continuous and batch processes has also been included.)

The procedure uses a depth-first, least-commitment strategy that attempts to complete a base-case design before we consider any alternatives, because we might encounter some decision at a later stage in the design that will make all of the process alternatives unprofitable.

Within each level of the hierarchy the decisions that need to be made have been identified and precedence ordered, so that the problem of conflicting subgoals is avoided. In addition, in Douglas' procedure,

TABLE 2
Hierarchy of Decision Levels

0) Input Information
1) Batch vs. Continuous
2) Input - Output Structure
3) Recycle Structure
4) Separation System
    a) Vapor Recovery System
    b) Liquid Separation System
5) Energy Integration
6) More Detailed Alternatives

heuristics (*i.e.*, qualitative knowledge) are used to fix the structure of the flowsheet, to identify the dominant design variables and to fix some of the secondary design variables, while algorithms (*i.e.*, quantitative knowledge) are used to calculate the process flows, the utility flows, the equipment sizes, and both the capital and the operating costs as a function of the design variables.

We use cost calculations to ensure that the process is profitable over at least some range of the design variables before we continue on to the next level in the hierarchy. If the process is unprofitable over the complete range of the design variables, then we use the previously identified backtracking points to examine the process alternatives. If a profitable alternative cannot be found, then we terminate the design project.

An initial evaluation of this hierarchical decision procedure was undertaken by teaching seventeen three-day short courses at various industrial sites. Normally twenty-five students with three to twenty

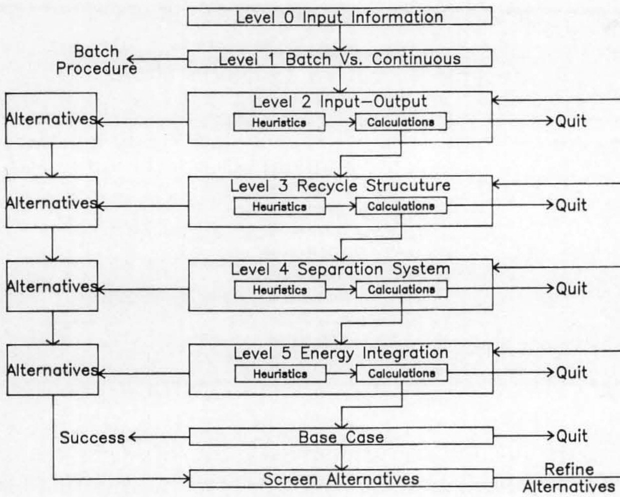

FIGURE 6. Flowchart of PIP operation

years of experience in design participated. The feedback obtained from these courses was used to modify the hierarchical procedure, but all of the students believed that the course was much better than the undergraduate course that they had taken. Many of the experienced designers had previously used some of the short-cut techniques that were presented, but all of them were surprised that such a systematic procedure could be developed.

An interactive computer code called PIP (Process Invention Procedure) based on Douglas' procedure for process synthesis has been described by Kirkwood [5]. The structure of the program is given in Figure 6, and the relationship between the qualitative knowledge bases and the quantitative knowledge bases, as well as the backtracking points, is indicated. This software makes it possible for an experienced user to complete a conceptual design in one to three hours and to find the best flowsheet alternative in about one day, for the limited class of processes considered.

The code was written for an IBM-PC/XT in order to make it simple for a variety of industrial companies to be able to evaluate the synthesis procedure on their own processes. The companies that have participated in this effort are: American Cyanamid, Du Pont, Exxon Chemicals, General Electric, Imperial Chemical Industries (UK), Mobil, Monsanto, and Tennessee Eastman. The evaluations have been generally favorable, with the main complaint being that the conceptual designs that were currently under investigation in those companies were for multiproduct plants, agricultural processes, or other processes that were beyond the scope of the code.

TABLE 3
Input Information Menu

F1 (HELP) Type the desired option and RETURN
F3 (SAVE) F4 (NEWSAVE)

INPUT INFORMATION
Review

1) Process Name
2) Primary Product
3) Reaction Information
4) Feedstream Information
5) Physical Property Date
6) Process Constraints
7) Plant and Site Data
8) Review All Input Information
9) Continue on to Decision Level Menu

PIP-PROCESS INVENTION PROCEDURE

The availability of the PIP program removes the tedious computational effort from the development of a conceptual design and the evaluation of process alternatives. Some additional details concerning the code are presented below, and more information concerning the structure of the code is given in a paper by Kirkwood [5].

Level 0—Input Data

The menu where the user enters the input data is shown in Table 3, and a set of responses for a process that will produce benzene via the hydrodealkylation of toluene are given in Table 4. Help screens are available for the appropriate formats for the input data. The available physical property data can be verified and default data for the utilities can be changed.

TABLE 4
Required Input Data for the HDA Process

The Primary Product is BENZENE
The Production Rate in Lb-mol/hr is 260.00
Its Purity in Mole Fraction of Product is 0.99
Does it form an Azeotrope? (Y or N) N
The Value of the Product Stream in $ / lb-mol is 9.04

REACTION INFORMATION

Reaction #	Reaction	Phase	Temperature (Deg. F.)	Pressure (Psia)
1	H2 + TOLUENE = BENZENE + CH4	VAPOR	1150.00	500.00
2	2.0 BENZENE= DIPHEN + H2	VAPOR	1150.00	500.00

FEEDSTREAM INFORMATION

Feedstream 1

Component Name	Mole Fraction
H2	0.96
CH4	0.040

VAPOR Pres = 500.00 Cost = 1.32

Feedstream 2

Component Name	Mole Fraction
TOLUENE	1.00

LIQUID Pres = 15.00 Cost = 6.40

Level 2—Input-Output Structure of the Flowsheet

For a continuous process, we then proceed to Level 2, the Input-Output Structure of the flowsheet. The menu is shown in Table 5. For the process under consideration, the heuristics included in the code indicate that it is not desirable to purify the hydrogen feedstream (the program noticed that the gaseous feedstream is not pure and a heuristic indicates that usually it is too expensive to purify gaseous feedstreams), that the feed of an excess of one reactant to the process would not normally be desirable, that the reversible by-product (identified by PIP as diphenyl) will be removed (this is a default decision), and that a gas recycle and purge stream is required (the code recognizes that the hydrogen reactant cannot be recycled without methane building up in the gas recycle loop). The user is required to verify these decisions, and a function key is available to explain the appropriate heuristic.

Heuristics are then used to determine the number of product streams and which components are in each. The user is then asked for the values (*i.e.*, fuel, by-

TABLE 5
Input-Output Structure Decision Menu

F1 (HELP)   Type the desired option and RETURN   F2 (HEURISTIC)
F3 (SAVE)   F4 (NEWSAVE)

INPUT - OUTPUT STRUCTURE
Review and Results
1) 1.1) Feedstream Purification
(N/A) 1.2) Excess Reactant Specification
1.3) Reversible Byproduct Destination
1.4) Light Component Destination
2) Component Classification
3) Product Distribution Data
3.1) Extents of Reaction
-OR-
3.2) Reaction Rate Equations
4) Process Constraints
5) Review All Input-Output Information
6) Results of Calculations
7) Return to Decision Level Menu

TABLE 6
Input-Output Result Menu

F1 (HELP)   Type the desired option and RETURN

RESULTS: LEVEL 2 INPUT - OUTPUT STRUCTURE
1) Design Variable Ranking
2) Flowsheet Picture
2.1) Simple Structure
2.2) With Flowrates
2.3) With Stream Costs
3) Case Study Optimization of Design Variables
3.1) Graphical Output
4) Process Alternatives
4.1) Alternatives to Consider
4.2) Current Process Decisions
5) Return to Level 2 Input Menu

TABLE 7
Recycle Structure Decision Menu

Type the desired option and RETURN
F3 (SAVE)   F4 (NEWSAVE)

RECYCLE STRUCTURE
Review and Results
1) Reactor Specifications
2) Recycle Component Classification
3) Molar Ratio Specification
4) Process Constraints
5) Review Recycle Structure Information
6) Results of Calculations
7) Return to Decision Level Menu

product, pollution treatment cost, *etc.*) of each stream. Finally, information about the product distribution for the reaction system is required. Either a correlation of the extents of the reactions as functions of the design variables or as a kinetic model may be specified.

Once this information has been entered, the user can proceed to the result menu for Level 2 (see Table 6). Using option 2.2, the value of the design variables are specified and then the code will generate a picture of the flowsheet with the total flows of each of the process streams (Figure 7). For option 2.3, after specifying values for the design variables, a flowsheet that shows the stream costs can be generated. Each of these calculations takes less than one second.

It is possible to examine the complete range of the design variables and see where the process is profitable by choosing option 3.1. Assuming that profitable operation is obtained over some range of the design variables, the program will proceed to the next level in the hierarchy of decisions. A list of the process al-

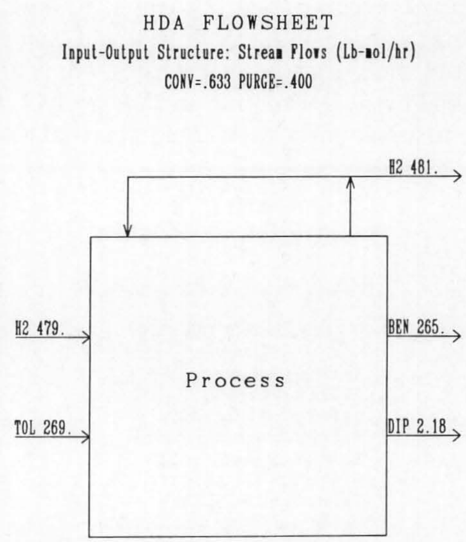

FIGURE 7. Input-output flowsheet with stream flows

ternatives that could be considered, *e.g.*, recycling the reversible by-product to extinction, can also be examined.

Level 3—Recycle Structure of the Flowsheet

The menu for Level 3 is given in Table 7, and the user is required to verify the number of reactor systems selected, the number of recycle streams generated, and both the limiting reactant conversion and the molar ratio of reactants will become new design variables (if applicable).

The result menu for Level 3 is shown in Table 8. The new flowsheet with annualized capital and operating costs (option 2.3) can be generated (see Figure 8). Option 3.1, a two-variable plot of the profit (economic potential) with the recycle costs included, is shown in Figure 9. Note how the range of the design variables where profitable operation is obtained has decreased

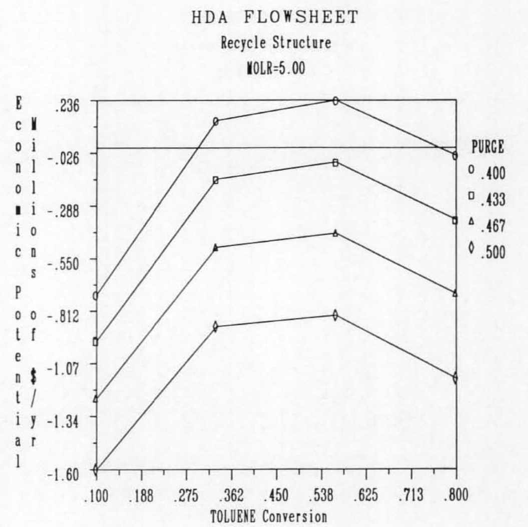

FIGURE 9. Recycle structure economic potential plot

significantly, simplifying the task of synthesizing a separation system. In addition, sensitivity studies of the effect of changing the gas recycle pressure drop (if any) and the reactor heat effects can be made (options 4.1 and 4.2).

TABLE 8
Recycle Structure Result Menu

Type the desired option and RETURN

RESULTS: LEVEL 3 RECYCLE STRUCTURE
1) Design Variable Ranking
2) Flowsheet Picture
    2.1) Simple Structure
    2.2) With Flowrates
    2.3) With Stream Costs
3) Case Study Optimization of Design Variables
    3.1) Graphical Output
4) Recycle Structure Process Unit Analysis
    4.1) Reactor System 1
    4.2) Recycle Compressor
5) Process Alternatives
    5.1) Alternatives to Consider
    5.2) Current Process Decisions
6) Return to Level 3 Input Menu

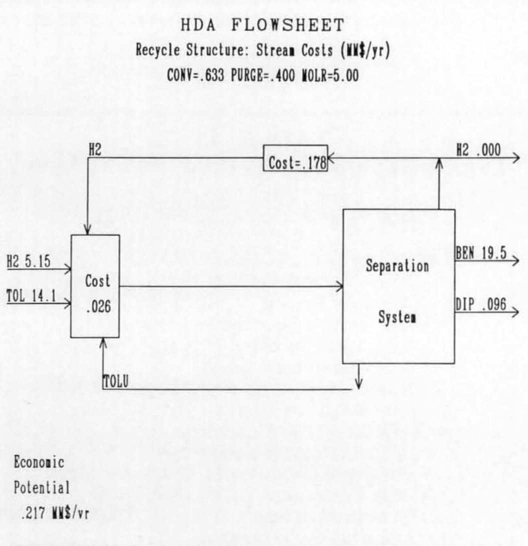

FIGURE 8. Recycle Flowsheet with economics

Level 4—Separation System

The menu for the synthesis of the separation system is given in Table 9. The phase of the reactor effluent stream is determined at the current optimum of the design variables where profitable operation is observed in Level 3, and a heuristic is used to fix the general structure of the flowsheet (see Figure 10). A flash calculation is then used to determine the component flows in the flash vapor stream (if one is present) and the value of materials lost in the purge stream. If these losses are significant, or if there are components in the gas recycle stream that would be deleterious to

TABLE 9
Separation System Menu

Type the desired option and RETURN

F3 (SAVE) F4 (NEWSAVE)

SEPARATION SYSTEM
Review and Results
1) Separation System Structure
    1.1) Reactor System 1
2) Separation Split Block
    2.1) Reactor System 1
3) Vapor Recovery System
4) Liquid Separation System
    4.1) Glinos-Malone-Nikolaides,
        Fenske-Underwood-Gilliland Model
        (i.e. short-short-cut)
    4.2) Fenske-Underwood-Gilliland Model
5) Return to Decision Level Menu

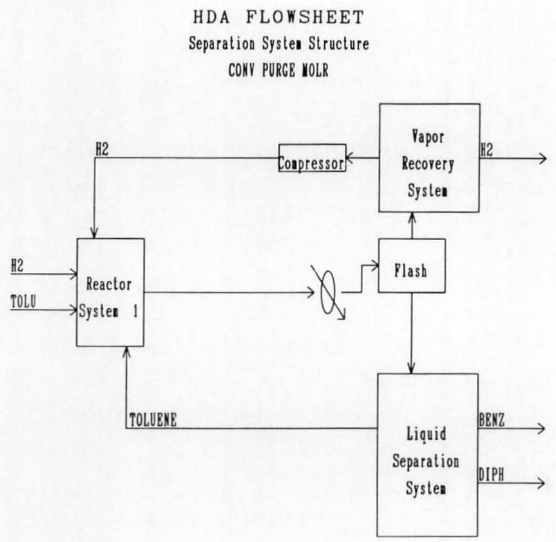

FIGURE 10. Separation system flowsheet

the reactor performance, the user can install a vapor recovery system (Table 10). Several types of systems and locations can be selected. In our example we do not include a vapor recovery system.

Next we consider the synthesis of a liquid separation system (see Table 11). Currently, distillation is the only separation process considered. We determine the best sequence by exhaustive enumeration (it takes about five seconds to complete this calculation). A flowsheet showing the best distillation sequence, the process flows, and the equipment sizes for the design variables indicated is presented in Figure 11. Detailed design information for each piece of equipment and each of the process streams is available by pressing a function key. The results of a one variable optimization study are shown in Figure 12, and again we see that the range where profitable operation is possible is significantly reduced.

Level 5—Heat Exchanger Network Synthesis

We use the procedure described by Hohmann [6], Umeda *et al* [7], and Linnhoff and Flower [8] to calculate the minimum heating and cooling loads for the process, and we use the surface area targeting procedure of Townsend and Linnhoff [9] to estimate the heat exchanger area required. With this information we can estimate the capital and operating costs of the heat exchange system. In addition, we add the minimum approach temperature to our list of significant design variables.

Evaluation of Process Alternatives

At this point we have completed a base-case design and obtained a reasonable estimate of the optimum design conditions. Hence, we return to our list of process alternatives, and we attempt to find a better flowsheet. We first consider alternatives that correspond to decisions where there were no heuristics available (*e.g.*, the recycle of reversible by-products), and then we consider alternatives that change the structure of the flowsheet at the early levels in the hierarchy.

By proceeding to Level 6 we can also evaluate the effects of alternate reactor configurations (plug flow-CSTR combinations, temperature profiles, and feed distributions), complex distillation column alternatives, and alternative heat exchanger networks. Hence, we can explore a number of alternatives with relatively little effort.

CONCLUSIONS

Teaching Process Synthesis

In the undergraduate design course, we describe each of the decision levels in detail, we discuss the heuristics that are available for making the decisions, and we derive the short-cut design equations that are used to calculate the costs. The base-case design for one process is developed in this way and a list of process alternatives is generated. Then the alternatives

TABLE 10
Vapor Recovery System Result Menu

Type the desired option and RETURN

RESULTS: LEVEL 4 VAPOR RECOVERY SYSTEM
1) Evaluate Vapor Recovery System Flows
2) Choice of Vapor Recovery System
    2.1) Adsorption
    2.2) Condensation
>> 2.3) No Vapor Recovery System
3) Flowsheet Picture
    3.1) Simple Structure
    3.2) With Flowrates
    3.3) With Stream Costs
4) Case Study Optimization of Design Variables
    4.1) Graphical Output
5) Process Alternatives
6) Return to Level 4 Menu

TABLE 11
Liquid Separation System Result Menu

Type the desired option and RETURN

RESULTS: LEVEL 4 LIQUID SEPARATION SYSTEM
1) Design Variable Ranking
2) Flowsheet Picture
    2.1) Simple Structure
    2.2) With Flowrates
    2.3) With Stream Costs
3) Case Study Optimization of Design Variables
    3.1) Graphical Output
4) Distillation Train Evaluation
    4.1) All Possible Sequences
    4.2) Best Sequence vs. Design Variables
    4.3) Define Liquid Separation System
5) Process Alternatives
6) Return to Level 4 Menu

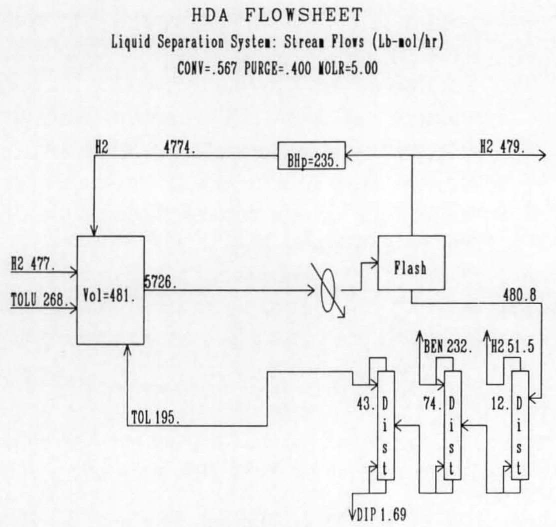

FIGURE 11. Liquid separation flowsheet with stream flows

are considered in an attempt to find the best process flowsheet. Moreover, the results of the short-cut calculations are compared to a rigorous computer-aided-design solution in order to evaluate the accuracy of the approximate calculations.

The homework assignments in the course focus the student effort on developing a base-case design for a different process in a step-by-step manner by hand, at least for the early levels. Stand-alone software (a program developed by Glinos and Malone [10], is used to synthesize and evaluate the distillation sequences, while data for the synthesis of a heat exchanger network is generated in part by hand and in part using a CAD package. The goal of these assignments is to

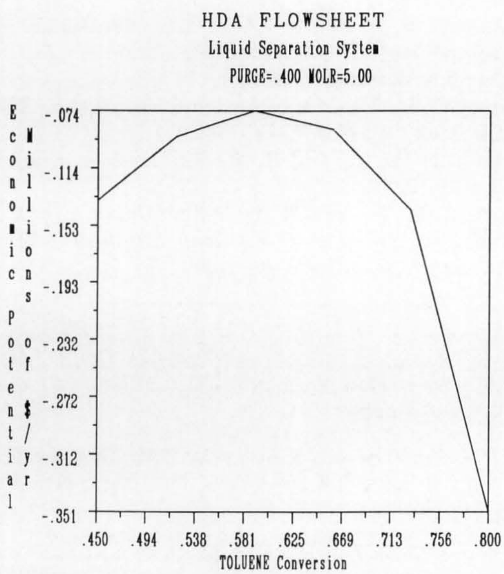

FIGURE 12. Liquid separation system economic potential plot

reinforce an understanding of the procedure.

Now that PIP is available we would introduce another set of homework assignments, which would be given in parallel with the development of the students' base-case design, that would explore process alternatives. This would allow students to focus their thinking on the physics and the economic trade-offs involved in the process and to minimize the amount of time they spend on calculations. Near the end of the course we would then give other assignments where the students would be expected to design new plants in a two-day time period. The focus in the class discussion would be on the similarities and differences between various types of processes.

SUMMARY

The current version of the software is applicable to a limited class of petrochemical processes, and we hope to extend it to solids processes, polymer processes, bio-processes, and batch processes. Research is underway to develop the necessary procedures. However, even in its present form we expect that it should provide a useful teaching tool.

We believe that it is possible to teach the conceptual design of chemical processes to undergraduates. Their lack of experience can be overcome to a great extent by providing new design tools and software which make very rapid calculations possible, so that even when they explore alternatives that *experienced* designers know would not be profitable, the time penalty will be small. The availability of the software also makes it possible for them to gain experience more rapidly.

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