

Burning Bright



Trends in Process Integration

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Process integration is more than just pinch technology and heat exchanger networks. Today, it has far wider scope and touches every area of process design. Switched-on industries are making more money from their raw materials and capital assets while becoming cleaner and more sustainable.

In the past, the major research emphasis in process design has been placed on the analysis, or simulation of processes. The synthesis of processes or process integration has, in comparison, received little attention. However, this is all changing. Until recently, process integration was virtually synonymous with pinch analysis and energy integration. However, over the past few years, there have been two significant trends that change this picture.

First, a wider range of solution techniques is now used. Rather than using only thermodynamic, or pinch methods, the advantages of mathematical programming and optimization have been combined. The insights from thermodynamics have been retained and combined with the power of mathematical methods for data handling, optimization and automatic design. The approach used as far as possible is to develop a deep understanding of the physical principles underlying problems, and only then to develop practical methodologies that employ the necessary mathematics.

As a result of the first trend, a much wider range of problems can now be addressed. Process integration can now be considered to cover four major areas — efficient

use of raw materials, energy efficiency, emissions reduction, and process operations. From these four research areas, we can see that process integration is far more concerned with material (mass) processing issues than in the past. Mass integration and energy integration, in fact, complement one another. This article will discuss how the two subjects are brought together in the latest research and development at UMIST.

Efficient use of raw materials

a) Design of novel reactor systems

For the design of industrial reactors, the most appropriate choice of configuration and mixing pattern, arrangements for feed and recycling of raw materials, and arrangements for handling the energy effects in the reaction system, have a critical effect on the performance of the reactor, and the process as a whole. The problem is made more complex by the fact that many reactors involve multiphase systems.

Design choices are often made on the basis of past experience or trial-and-error using laboratory tests and repeated simulation. Very often, a reactor is chosen because

it reminds designers of a similar system, because it has been used before, or simply because there is no time to search properly. Heuristics and expert systems can help, but these will often lead back to conventional designs.

A methodology has been developed for the systematic design of chemical reactors that sets performance targets, predicting the maximum yield and selectivity for a given reaction system with its catalyst (1). The technology was developed specifically to address industrial reactor problems, rather than academic ones.

This method owes far more to mathematics than to thermodynamics and is a good illustration of the use of newer tools. A superstructure consisting of generic reactor units and a network of interconnected streams that account for different layouts, arrangements and mixing patterns is created. This is then subjected to stochastic optimization or mathematical programming to give a target for the theoretical best performance (e.g., conversion, yield, selectivity, cost, etc.). However, many physical insights must be included in the problem formulation to obtain solutions.

Even the most complex systems can be analyzed, involving multiphase reactors and complex heat-transfer arrangements. When dealing with multiphase systems, a network is constructed for each phase and these are linked using an understanding of mass transfer. The mixing patterns and heat-transfer arrangements associated with the target provide the basis for the design to achieve the goal. Optimum catalyst distribution patterns can also be predicted. For new processes, the technology is capable of identifying the optimal reactor configuration and operation. For existing processes, it can be used to determine the potential for modifying the design.

The application of the technology leads to the development of novel reactor schemes that would be virtually impossible to derive using an approach based on trial-and-error. The technology has either led to designs with significant improvements in the yield of the process when compared with those based on conventional reactor designs, or reduced capital investment. This approach does not simply give one solution as being "the optimum." Rather, it provides the designer with a range of targets and design options.

The power of the approach can be illustrated with a study involving the chlorination of butanoic acid to form α -monochlorobutanoic acid (MBA) and an undesired byproduct, α - α -dichlorobutanoic acid (DBA). The objective is to maximize the yield of MBA. This is a difficult problem because first, there are two phases — gas and liquid — and second, the reactions and kinetics are complex. Further details are given elsewhere (2).

Let us consider the performance of three of the most widely used conventional gas/liquid reactors, namely: a packed-bed reactor, a mechanically agitated reactor and a bubble-column reactor (Figure 1). The mechanically agitated

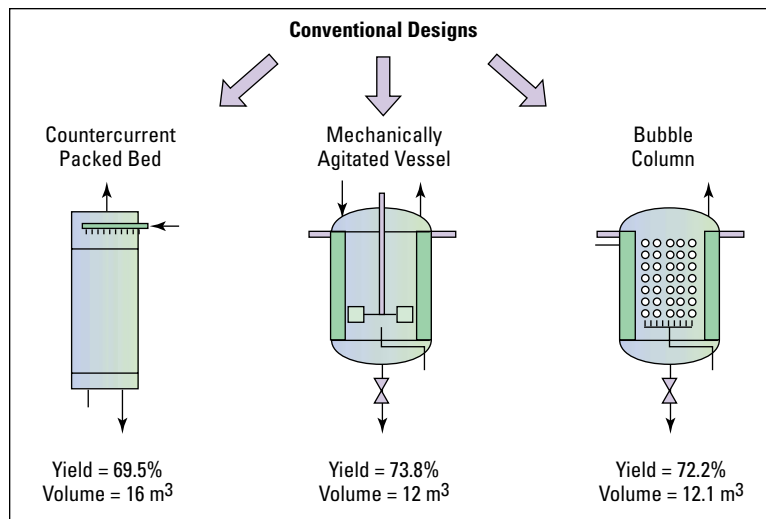


Figure 1. Conventional reactor performance for the chlorination of butanoic acid.

reactor has the apparent highest yield at 73.8% and would probably be selected for the application. However, optimizing the problem using the new methods — and without any commitment to a preferred- or conventional-reactor type — gives the design shown in Figure 2a. This has an MBA yield of 96.9%, which is a step-change in performance, compared with the conventional designs. Note the reactor volume is smaller than those of the conventional designs. Of course, the design in Figure 2a is an ideal situation, which must then be translated into a workable design. Two possible practical designs are shown in Figure 2b.

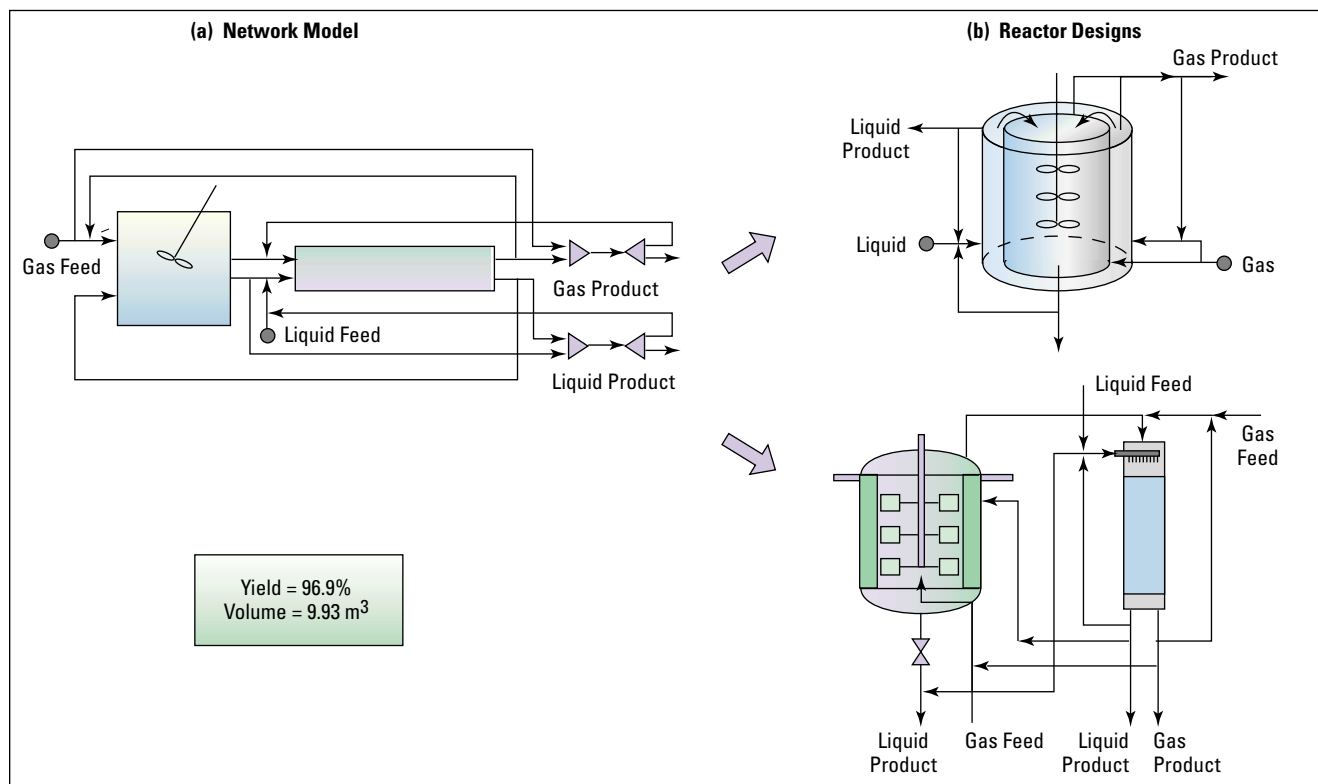
b) Design of reactor-separator-recycle systems

In most chemical processes, the effluent from the reactor is separated into products, byproducts and unreacted feed. The unreacted feed can be recycled back to the reactor system. Until recently, very few systematic procedures have been proposed for the synthesis of reactor-separator-recycle systems. A newly developed approach proposes a general superstructure of different reactors and separation tasks and features all the potential interconnections among the proposed units. The approach has highlighted the importance of the coupling between the reaction and the separation system and confirmed the potential benefits of an integrated approach (3).

c) Reactive distillation

Reactive distillation not only removes a step in a flow-sheet by carrying out two operations in one unit, but also allows reactions with unfavorable equilibria to achieve higher reactor conversions and to improve reaction selectivity. The design issues in reactive distillation are much more complex than in conventional distillation. Both homogeneous and heterogeneous catalysts can be used. In some applications, the whole column is reactive. In others, only part of it is reactive with conventional separation occurring in the non-reactive zones. Many design options are possible with different feed and product take-off arrangements. Intermediate heating and cooling can be carried out and recycles between different parts of the arrangement might be advantageous. This research identifies the optimal structural configuration and operating conditions for reactive distillation (4). Again, a more mathematical approach is adopted to deal with the complexi-

Process Integration



■ Figure 2. A novel solution shown as (a) network representation and (b) real reactor systems.

ties of such problems, incorporating physical insights into the problem formulation.

d) Design of solvent-based separations

Previously, the selection of solvents has normally been left to experience or trial-and-error. A new approach has been developed for designing separation agents (5). Representing materials as a combination of functional groups identifies promising molecular structures. The most appropriate combination of functional groups is optimized to give material with the most desirable properties. Once a solvent has been selected, a flowsheet structure needs to be developed. The appropriate configuration with its recycles has a profound influence on the efficiency of the process and the potential for solvent losses. Systematic methods are being developed for the design of such solvent-based separation processes. This includes the design of optimal mass-exchange networks, which are systems of separators that use mass-separating agents to selectively transfer certain species from process streams (6, 7).

e) Hydrogen integration in petroleum refining

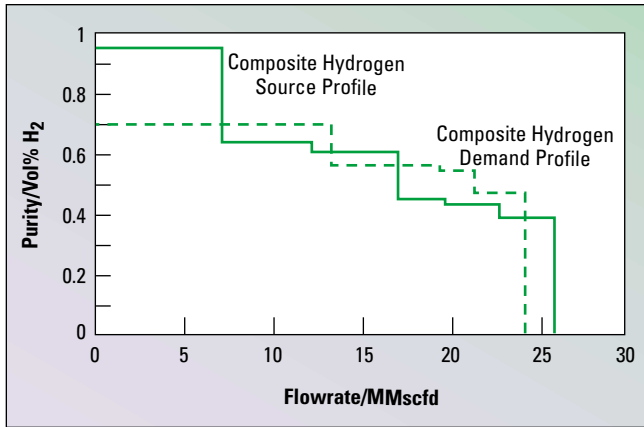
Until recently, hydrogen availability was not a major issue for most refineries. In fact, many plants had hydrogen to burn ... literally! Most hydrogen systems in existing refineries feature little or no integration. Several trends in the oil industry are leading to an increased demand for hydrogen in refineries and this changes the picture drastically. First, stricter legislation on sulfur content in fuels increases the need for hydrotreating. At the same time, regulations on gasoline aromatics composition are constraining reformer operation and removing some of the sources of hydrogen traditionally available to refineries. Second, the move to processing of heavier crude oils and the reduced market for heavy fuel oil

is forcing greater use of hydrocracking for upgrading. Simply increasing the throughput of a refinery will also lead to increased hydrogen requirements, with the existing hydrogen production capacity often being a bottleneck.

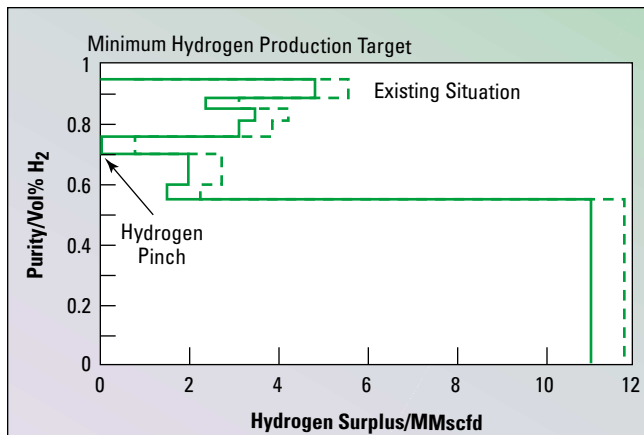
A methodology has recently been developed for assessment of hydrogen resources, based on an analogy with the problem of process heat recovery (8). This method constructs hydrogen composite curves, showing the demands and sources of onsite hydrogen in terms of stream purities and flowrates (Figure 3). This is used to construct a hydrogen surplus diagram (Figure 4), which is analogous to the grand composite curve for energy systems. This diagram allows the engineer to find the "hydrogen pinch" and to set targets for hydrogen recovery, hydrogen plant production and import requirements.

This method also gives insights into the effective use of hydrogen purification units. It has been shown that a purification unit (*e.g.*, a pressure-swung adsorber, a membrane or a cryogenic separator) should not be placed below the hydrogen pinch. Purifying gas above the pinch may have some benefits, but placing the purifier across the pinch is the best option (8).

The pinch approach is useful for conceptual purposes, but has some limitations when applied to real systems. For example, it does not take account of stream pressures, and thus assumes that any source can be fed to any sink, even if there is insufficient pressure. An improved approach has recently been developed (9) that can account for pressure and makes best use of the existing compressors in a refinery. This method is mathematically based and can account for all important costs and tradeoffs including hydrogen production, compression power, fuel value, and piping costs. It is well suited to both new design and retrofit studies.



■ Figure 3. Hydrogen composite curves.



■ Figure 4. The hydrogen surplus diagram is used to target the minimum supply requirement. The dashed profile shows the existing case, which is unpinched (i.e., uses excess hydrogen). The supply flowrate is reduced until the surplus diagram just touches the vertical axis (i.e., becomes pinched). This is the minimum feasible flowrate.

The new technology can be used to achieve several objectives. First, it can be used simply to save hydrogen, and hence reduce the costs associated with its production. It can also be used to meet new fuel specifications with a minimum level of capital investment. Similarly, it can be used to increase the refinery throughput, as well as to provide the flexibility to process various oils and to change the product spectrum for improved profitability.

f) Integrated combined cycle gasification processes

As a result of the worldwide trend towards stricter environmental regulations and increased demand for better quality products, integrated-gasification-combined-cycle (IGCC) technology has become an attractive option for the refining industry. Gasification converts the “bottom of the barrel” into valuable products such as hydrogen, clean fuel, and power. The major issues involved to establish an IGCC as an economically viable process include selection of the best IGCC feedstock and better use of existing facilities. Methods have been developed to identify and remove bottlenecks to enhance throughput, and also to optimize the unit connections, allocation of utilities and operating modes. This is aimed at increasing refinery economic margins.

Energy efficiency

Much work in this area involves separation systems, with distillation being the most significant. Others are still concerned with heat recovery and utility systems, but now make far more use of mathematical methods than was previously the case. Specialized methods for retrofit have been developed.

a) Design of complex distillation systems

It has become clear in recent years that complex column arrangements can significantly reduce distillation costs compared to systems comprising only simple columns (columns with one feed and two products). Complex arrangements include pre-fractionators (and pre-flashes), side strippers, side rectifiers and fully thermally coupled (Petlyuk and dividing wall) columns. Once these options are included, the number of possible configurations to be considered explodes, and solving the problem by exhaustive enumeration becomes out of the question, even for small numbers of products. In addition, if thermal coupling is applied, this introduces further constraints into the problem.

A screening method has been developed that allows promising structures to be synthesized for distillation systems ahead of any detailed design or simulation. It allows systematic development of performance targets and automated development of novel designs (10).

This approach is based upon a new representation, which incorporates all possible design alternatives. Figure 5 shows how this representation is used to synthesize sequences of simple columns to separate out five components. Note that discrete “tasks” are used instead of units and/or networks. All possible simple-column sequences can be generated from this representation. For example, the direct sequence (i.e., where the lowest-boiling component is removed in each column) can be generated by selecting tasks 1, 8, 15 and 20, in that order.

As shown in Figure 5, complex column configurations can be derived by forming hybrids of separation tasks. This can be extended to systems performing sloppy or non-sharp separations by including more tasks in the hybrids. Where column pressure is another degree of freedom, this can be dealt with by introducing clone tasks at discrete pressure levels for all simple and hybrid tasks.

The reason for using the task representation is that a combination of tasks (supertask) is easier to model than a composite network of sequences. Also, the number of possible tasks increases much slower than the number of possible sequences when the number of components to be separated increases. This prevents the problem size from exploding.

Shortcut column calculations and cost correlations are used with a mixed-integer linear program (MILP) to generate a spectrum of cost-effective designs. Both capital and operating (energy) costs can be considered in the objective function. Promising structures can then be subjected to more detailed simulation and design.

A case study supplied by M.W. Kellogg will be used for illustration. This problem involved the separation of the effluent from a catalytic reformer. There were 22 components

Process Integration

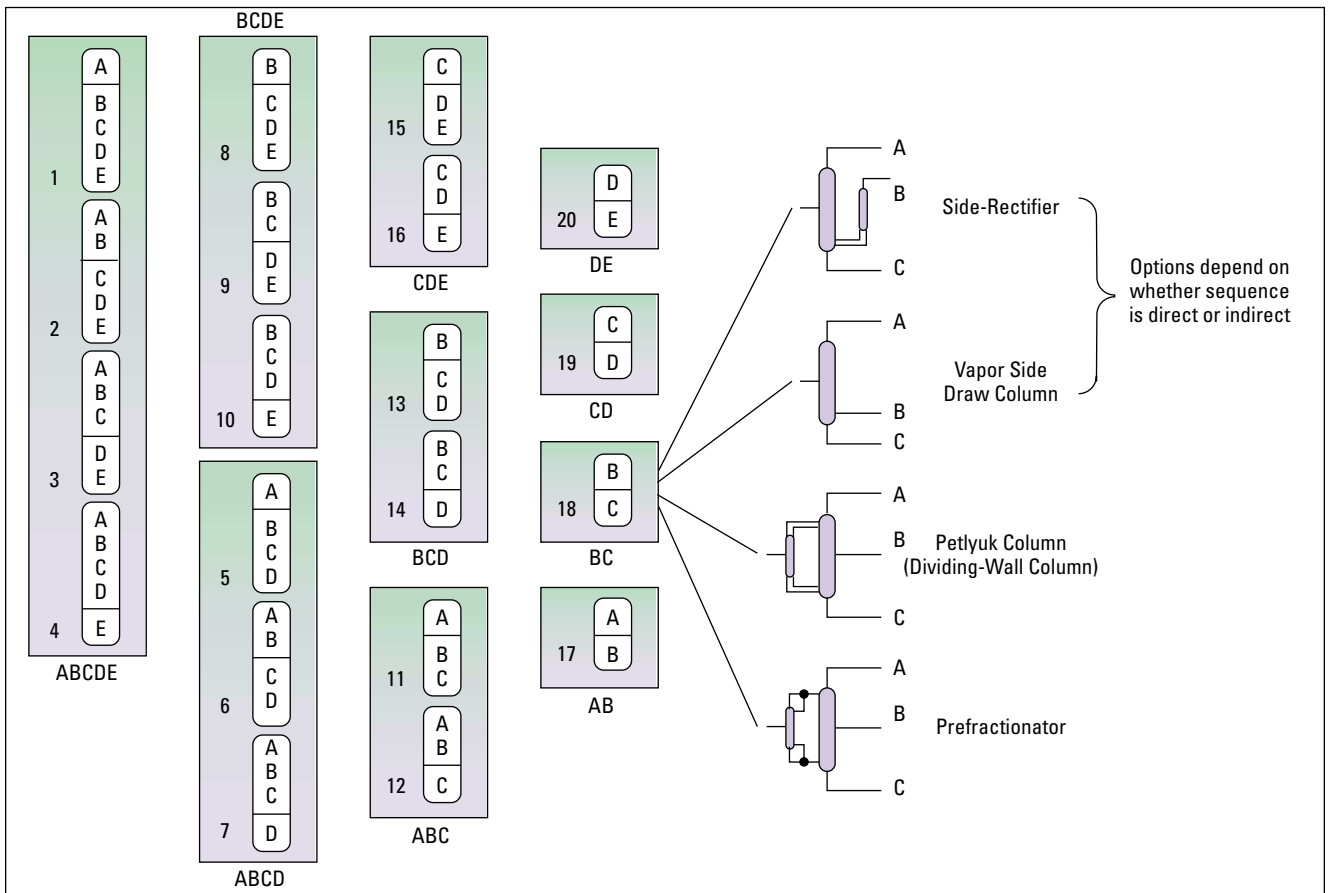


Figure 5. A five-component separation problem shown as a task representation. Tasks can be merged to form hybrids to allow for complex configurations.

in the mixture and the product streams were also to be multi-component. The new method generated the spectrum of design alternatives (Figure 6) in under two minutes of computer time, even though the number of components was large. The solutions are ranked in terms of energy cost, and it can be seen that they all offer significant benefits over the best sequence of simple columns. This approach has also been applied to sub-ambient systems, such as ethylene cold-end separation, to give significant reductions in the refrigeration shaftwork requirements (11).

b) Dividing-wall distillation columns

The dividing-wall column is a fully thermally coupled design, which combines a prefractionator with a main distillation column in a single shell. It has been established that energy savings of 30% are typical because of the prefractionation effect. In addition, the dividing-wall column can, in new designs, save up to 30% of the capital cost compared with a conventional arrangement. Despite these benefits, industry has largely been reluctant to exploit this technology because it is unconventional. Until recently, there was a lack of reliable design procedures and a

fear of control and operational problems. New design methods have recently been established (12) for fully thermally coupled designs that optimize the design for minimum energy consumption and allow initialization for rigorous simulation. They also consider the heat integration potential of the configurations, as well as the implications for control.

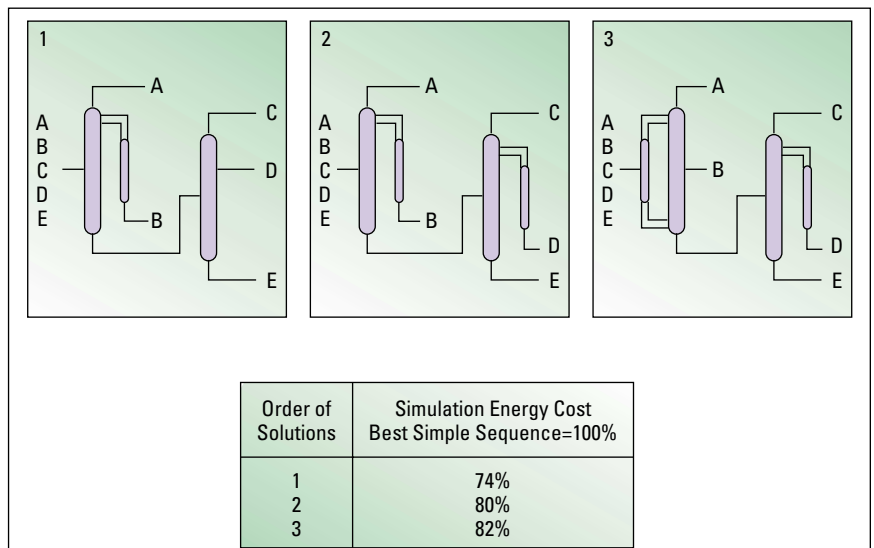
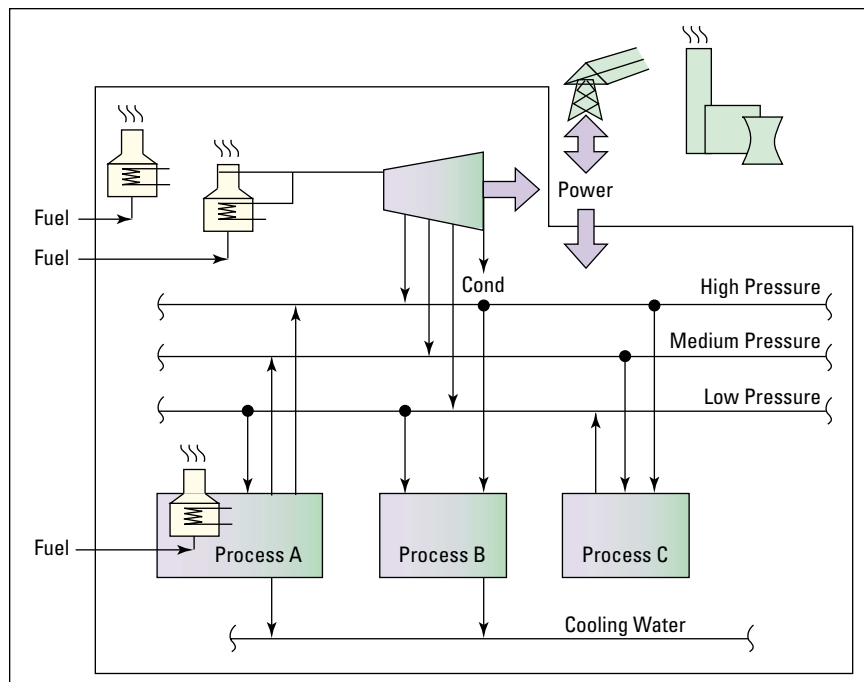


Figure 6. Spectrum of design options for the catalytic-reformer effluent separation problem.



■ Figure 7. A total site in which a number of processes are linked to the same utility system.

f) Cogeneration and site utility systems

Processes operate in the context of a total site, in which a number of processes are linked to the same utility system (Figure 7). The utility systems of most sites have evolved over many years without fundamental questions being addressed as to the design and operation of the utility system. The picture is complicated by the growing trend of individual production processes on a site belonging to different business areas, each assessing investment proposals independently of one another and each planning for the future in terms of its own business. Yet the efficiency of the site infrastructure and the required investment is of strategic importance and must be considered across the site as a whole, even if this crosses the boundaries of different business areas.

c) Separation of azeotropic mixtures

Many industrial distillation problems involve mixtures that form azeotropes. Several methods can be used to break the azeotrope, of which the most common is to add a mass-separation agent, known as an entrainer. The choice of entrainer depends on the phase-equilibrium behavior of the system. Pioneering work in the area of azeotropic distillation design includes that of Doherty, Stichlmair, Wahnschafft and others. A comprehensive review is given by Widagdo and Seider (13).

More recent work at UMIST (14, 15) has developed automated design methods for the synthesis of azeotropic-distillation sequences. These consider mass-transfer rates, as well as equilibrium, and can create new possibilities for column sequences that require less energy and lower entrainer flows. The techniques developed can be applied to any mass-transfer model or method of azeotropic-distillation sequence design.

d) Thermodynamic analysis of distillation

Once the structure of the separation sequence has been determined, thermodynamic analysis can be applied to individual separators to improve both their inherent efficiency and their heat integration potential (16). The methods can now be applied to all types of column design, including columns with multiple feeds and side-draws and side strippers/rectifiers. Even the most complex arrangements, such as those used in petroleum refining, can now be analyzed (17).

e) Design of absorption separation systems

Physical absorption is the most commonly used alternative to distillation for the separation of light gases. Chemical absorption is an important operation for the separation of acid gases. New arrangements have been developed for the separation of acid gases to achieve extremely low outlet concentrations at low capital and energy cost, removing the need for downstream treatment (18). These include several different double-loop arrangements.

Total-site pinch analysis provided an overall picture of the site and utility system (2), and allowed targets to be set for utilities, fuel, emissions, cooling and cogeneration. This approach, however, does not completely account for the interactions between improved heat recovery on an existing site and the efficiency of cogeneration. A new site revamping methodology, top-level analysis (19), has recently been developed to achieve this.

The original methods for site analysis required heat exchange data for every individual process and the data extraction for the entire site, which could take several months to obtain! Also, the methods often led to projects that could not be implemented because of constraints in the utility system. Finally, an expert user was needed to carry out the analysis.

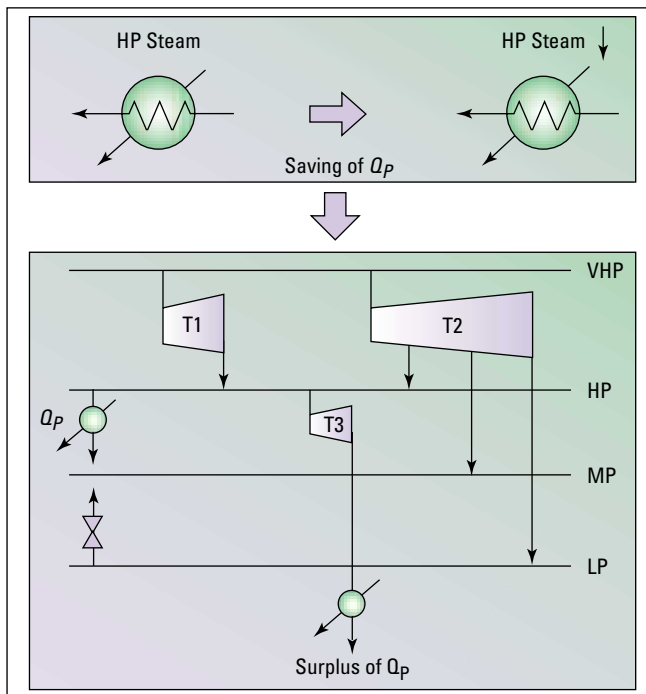
In top-level analysis, the problem is literally flipped upside-down and uses the following strategy:

- Start with the utility system to establish the scope for improvement and economic directions in terms of specific energy saving targets, then
- Use the economic directions to undertake process heat-exchanger network retrofits and identify projects with minimum capital investments.

The procedure requires only utility data to begin with, which can usually be gathered in a matter of days. Once this has been obtained, the analysis then looks at the benefits that would be achieved by saving a certain utility (for example, steam at a particular pressure) in the processes. These energy savings cannot be directly converted to fuel savings, and therefore cost savings as they can result in lower power generation on the site. Therefore, the trade-off between fuel consumption and power generation needs to be studied.

To illustrate, consider the utility system shown in Figure 8. We would like to know the benefit of saving an amount, Q_p , of high-pressure (HP) steam. As the diagram shows, this would result in a surplus of Q_p in the HP steam header. There are two

Process Integration



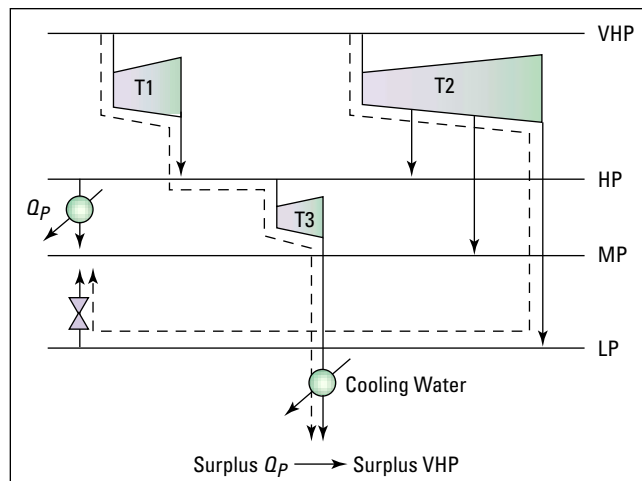
■ Figure 8. Saving Q_p of HP steam means that there is a surplus in the steam header. How can we best exploit this surplus?

ways to exploit this surplus. It can either be saved (giving a fuel saving), or it can be used to generate extra power. Which is the better option will depend on fuel costs, power costs and the efficiency of the power-generation equipment. All the possible heat flow paths in the utility system are then analyzed, and the surplus heat is shifted among these paths to find the most efficient option (Figure 9). Note that limits on the utility system hardware are included here.

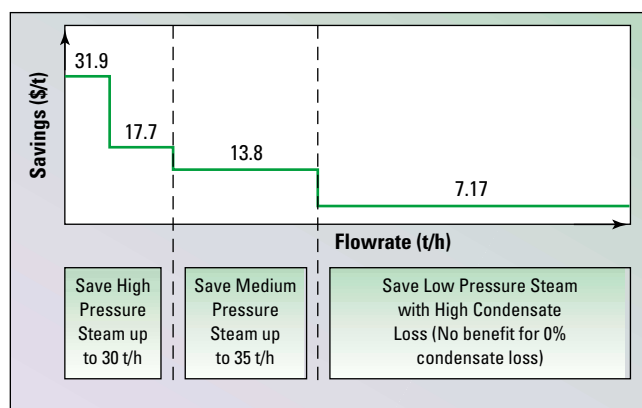
This analysis is carried out for all the utility levels and the results used to construct a financial benefits chart (Figure 10). This sets out which steam levels are worth saving. It gives the maximum potential and financial benefit for saving steam and also includes the turbine performance and limitations. In the diagram, we see that HP steam is the most worthwhile to save and that a maximum saving of 30 t/h is possible or economic. We see that we should then turn our attention to saving medium-pressure (MP) steam, this time up to 35 t/h. It also shows that saving low-pressure (LP) steam is not worth much, especially if the existing condensate return-system is efficient.

Having found the correct directions, we can then extract the heat-exchanger-network data judiciously. We need only consider processes using HP and MP steam. Bearing in mind that heat-exchanger-network data are by far the most time-consuming to gather, this approach can save weeks or months of effort. Once this is done, methods exist for achieving the steam savings, either by switching steam in utility exchangers or by improving the process heat recovery (20).

New tools have also been developed to determine the most appropriate number and levels of steam for the site, and, simultaneously, the most appropriate cogeneration system of steam turbines and gas turbines. The total site technology can



■ Figure 9. Steam of a given level can be produced by several different routes or paths, which link boilers, turbines and throttling valves. We can improve the performance of the utility system by maximizing steam flow through the most efficient paths. This figure shows an example of two paths.



■ Figure 10. The financial benefits chart shows which steam levels are most worth saving.

be used to reduce operating costs for an existing system, to determine and assess new investment proposals or to provide long-term investment plans for the infrastructure to allow for projected changes in the pattern of production.

g) Design of cooling-water systems

The use of recirculating cooling-water systems is the most common method employed to reject waste heat to the environment. The majority of designs use networks of cooling-water coolers that operate in parallel. Novel arrangements allow lower recirculation rates and better cooling tower performance. In debottlenecking situations, where cooling tower capacity is limiting, it can allow increased throughput without investment in new cooling tower capacity. New methods have been developed for the design of cooling networks. Coupled with new models for the cooling tower, the interactions between the design of the cooling tower and the cooling network can now be explored systematically.

h) Design of low-temperature systems

The operating costs for low-temperature (sub-ambient) processes are usually dominated by the cost of power to run the refrigeration systems. New methods have been developed recently to predict power requirements for refrigeration sys-



tems prior to design to within 3% of a detailed simulation. The approach works for all refrigerant fluids and for all of the complex features found in refrigeration systems (e.g., multiple levels, subcooling, economizers, pre-saturators, intermediate heat rejection, etc.). Multiple levels of refrigeration and cascaded systems can also be considered. Even mixed-refrigerant compositions can now be optimized to achieve minimum power in mixed-refrigerant systems (21).

i) Automatic design of heat-exchanger networks

It is well-known that rigidly following the pinch design method for heat-exchanger networks can lead to designs that are overly complex and potentially difficult to operate and control. This is not surprising, since the pinch method is based on thermodynamics only and is essentially aimed at minimizing energy consumption. It is difficult to include considerations, such as constraints and equipment limitations, in a thermodynamic approach, and it is understood that the design method would need to be tempered with an engineer's insight, judgment and common sense. Some attempts have been made to modify the pinch method, but these were all essentially still thermodynamic methods and suffered from the same inherent limitations. Incorporation of mathematical optimization was needed to avoid letting the "pinch" pinch us. The challenge has been to do this without letting the numbers crunch us.

A new, practical method has been developed for the automated synthesis of new heat-exchanger networks. This approach is based on a concept known as block decomposition (22). This concept uses physical insights from pinch analysis and decomposes the composite curves into a number of blocks, such that the streams in each block have similar characteristics. Each block will usually encompass several sections of the composite curves. In each block, a superstructure represents the possible matches between streams. As a result, the combined superstructure for the overall problem is much simplified, and thus the dimensions of the mathematical models are greatly reduced. The superstructure is then subjected to optimization, which allows the automatic generation of optimal or near-optimal networks with a low number of units.

This new technique not only significantly enhances design capability, but also allows for interaction. The designer has full control over network complexity to avoid impractical designs. In addition to trading off energy and capital costs, the new method allows for multiple utilities, constrained matches, variable heat-transfer coefficients and different cost laws for exchangers, producing designs that combine low costs with simple structures.

j) Retrofit of heat-exchanger networks

Traditional industrial practice has been to use pinch analysis concepts, or a variation of these, to retrofit heat-exchanger networks. However, this is not ideal as these methods in one way or another treat retrofit as a "pseudo" new design. This does not account for the existing layout and equipment limitations.

New methods have been developed that are quite different from previous approaches in that the design starts from

the existing network, rather than from the stream data. New approaches to retrofitting have been developed that automate the procedures using a combination of thermodynamics and mathematical programming. One approach that has been successfully applied in industry locates the network pinch, which is the bottleneck on heat recovery in the existing network structure (23). This is not the same as the original pinch and actually corresponds to a heat-exchanger unit in the system. Structural changes to the network are required to overcome the network pinch. The retrofit design proceeds one modification at a time from the existing network (23). In this way, the designer can develop retrofit projects in full control with the number of network changes (e.g., adding a new exchanger, exchanger relocation, stream splitting etc.) kept to a minimum.

k) Heat-exchanger-network design using intensified heat transfer

Heat-transfer operations can be intensified through the use of compact heat-exchangers and the use of heat-transfer enhancement techniques in conventional exchangers. The use of heat-transfer enhancement in heat-exchanger-network retrofit is well established. Retrofits often call for increased heat-transfer area on existing units, which can, in principle, be achieved using heat-transfer-enhancement techniques. We are now able to examine the use of intensified heat transfer as part of the overall approach for network design, such that it is used in a completely systematic way (24).

l) Power station design

The design of stand-alone power plants is significantly different from the design of cogeneration power plants. In the design of stand-alone plants, the efficiency of power generation is of paramount importance, and even small percentage improvements are important. Such a design is normally carried out by experienced power-station designers, making extensive use of simulators to evaluate designs. A new systematic methodology has been developed that uses a combination of thermodynamic analysis and mathematical programming for the conceptual design of power stations. Both new design and retrofit are considered. Applications have included gas-turbine integration into existing power stations (25).

Emissions reduction

These days, it is not possible to work in the chemical process industries and not have to consider environmental issues. CFC's, global warming, acid rain, carbon taxes and water pollution are but a few of the issues that are recognized as being critical.

a) Water system design

In the past, water has been assumed to be a limitless low-cost resource. However, there is now increasing awareness of the danger to the environment caused by over-extraction of water. As a consequence, the price of freshwater for the process industries is escalating. In some locations, it is likely that future increases in its use will be restricted. At the same time, the imposition of ever-stricter discharge regulations has driv-

Process Integration

en up effluent-treatment costs, requiring capital expenditure with little or no productive return. There is now considerable incentive to reduce both freshwater consumption and wastewater generation.

Water consumption can be minimized by maximizing the reuse of water. The approach is based upon analogies between heat transfer and mass transfer. Figure 11 illustrates how various water-using processes can be combined to give a composite curve for the whole system, allowing targets to be set for minimum water supply. These targets can be met by following certain rules that give a network design (Figure 12).

This conceptual work opened up an entirely new chapter for pinch analysis, but the original approach very rapidly ran into problems. First, it is difficult to extend this method to deal with multiple components. The two-dimensional graphical method works very well for heat transfer where there is only one transferred quantity (namely energy), but real water-systems feature several species that are transferred simultaneously.

Also, flowrate constraints (*i.e.*, processes that demand a fixed or minimum flowrate) are also difficult to account for. Another problem is that of operation modeling. Some operations, for example absorbers, can be modeled as having a fixed mass-transfer load. However, other operations, such as reactors or hosing operations cannot be modeled as primarily mass-transfer operations. Add to this the need to include practical constraints (*e.g.*, forbidden matches, forced matches, complexity constraints, etc.), as well as capital costing (*e.g.*, for pipes, sewers, treatment plants, etc.), and the simple water pinch approach simply cannot cope.

A recently developed approach uses mathematical programming. Firstly, each water-using operation is described by a model, which can be different for different contaminants. Then, a superstructure containing all possible connections is set up as shown in Figure 13a. Note that this structure includes all conceivable use, reuse, recycling and discharge alternatives. This is then optimized as a mathematical program, which is usually a combination of an MILP and a non-linear program (NLP). This gives an optimum network design as in Figure 13b. Details of the optimization are given elsewhere (26). This approach can handle all of the difficulties mentioned earlier, which the pinch approach could not. Further, the use of mathematical programming does not mean that the insights from the graphical method need to be sacrificed. It has been shown (26) how the output from the optimization can be used to build up a composite curve for the water system, thus retaining the graphical representation.

The chemical process industries make extensive use of hot water for washing and sterilization operations. Thus, it is most effective if energy and water management are considered together. Methods now exist for simultaneous energy and water

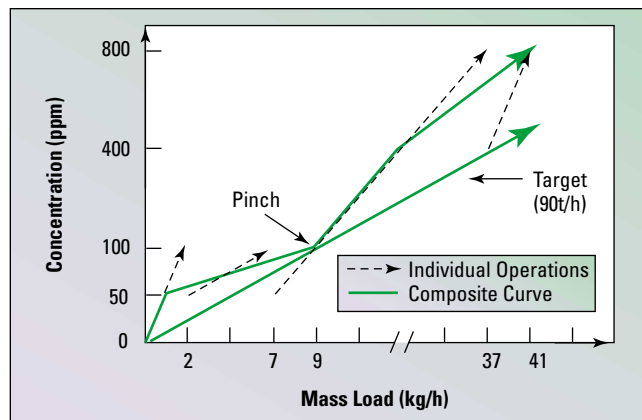


Figure 11. In the graphical water-pinch approach, the individual operations are combined to give a composite curve. The minimum water target is given by the inverse slope of the steepest line that can be drawn against the composite curve.

minimization (27). These consider isothermal and non-isothermal mixing of water streams with indirect heat recovery to ensure that energy and water targets are met with the simplest possible design.

Effluent treatment can also be handled. A similar approach can be used to design optimum treatment processes for a set of effluent streams. The essence of the method is to use distributed treatment instead of centralized treatment. In this approach, effluent streams are combined for treatment where necessary, but segregated if appropriate. This can reduce the volume to be treated and hence the cost.

More recent work has considered the water-use and treatment networks as one total water system. This is important because water treatment does not have to be limited to effluent streams. A treatment process can be used instead to regenerate water, so that it can be reused or recycled within the water-use network. Once again, a superstructure approach is used, but this is now a far more comprehensive and complex structure. As before, all relevant costs and constraints can be included.

b) Minimization of flue-gas emissions

Environmental concerns now require that the flue-gas emissions resulting from the supply of energy to processes should be minimized. A method now exists for a site utility-system design to meet the appropriate discharge regulations at minimum cost (28). This uses a combination of physical insights and mathematical programming, and is used to find the best strategy, which will be a combination of: changing fuel, modifying the utility system, process changes, improved heat recovery, cogeneration and chemical treatment. The em-

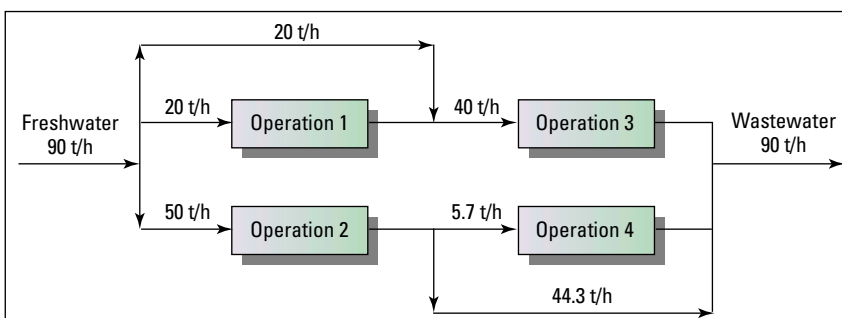
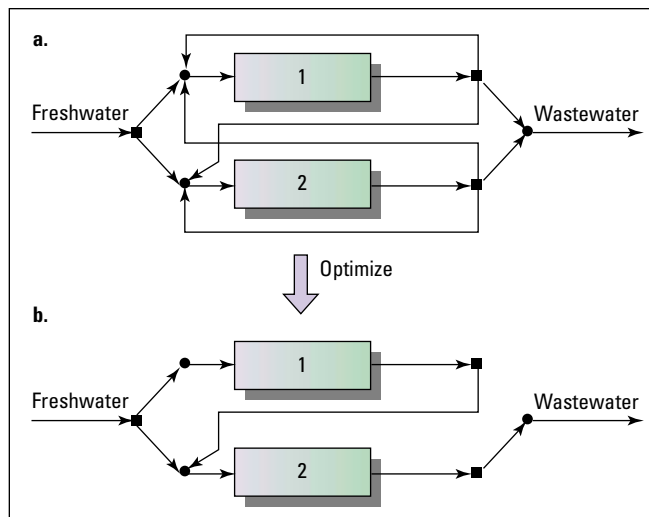


Figure 12. One possible network design to meet the target of 90 t/h.



■ Figure 13. (a) Superstructure for two water-using operations and one freshwater source. (b) Final design following mathematical optimization.

phasis is on achieving flue-gas limits with lower capital investment compared with conventional approaches, and potentially making operating cost savings at the same time. Both new designs and retrofits are considered.

Process operations

Early process integration work was concerned largely with conceptual design and did not really concern itself with day-to-day operations and planning. Now, however, major contributions have been made in these areas too.

a) Process optimization for commodity chemicals

A significant problem with the design and optimization of commodity-chemical processes is that the prices of feeds and products fluctuate over time. This project provides an analysis that is simple to carry out and can be used to design flexible processes that achieve maximum profitability under a wide range of conditions. Variations in prices are represented in a simple, graphical manner that rapidly identifies the economic conditions that a process is likely to encounter, while eliminating the need for price forecasts. This can be used to suggest alternative designs that offer flexibility if certain conditions are likely to occur. It can also be used to find the optimum capacity for a new plant and the optimum size of expansion for an existing one (29).

b) Refinery optimization and debottlenecking

A petroleum refinery is extremely complex. Profitable operation of a refinery requires an optimization of stream flows and process feeds. Most crude oils offer considerable flexibility in cut points, and many refineries are also able to handle a number of different crude oils. The optimization of the stream flows is constrained by the capacities of the equipment and by the desired specifications of the products. A new methodology has been developed involving three levels of analysis and optimization that takes into account all of the utility and process interactions (30). The refining processes, heat-exchanger networks, utility systems and hydrogen networks are all considered as one system. The aim is not simply to save energy or hydrogen, but rather to use these more efficiently to improve profitability. This can take the form of throughput increases, better product slates, or reduced feedstock costs.

Current operations are first optimized using models of the operations that allow for discrete (on/off) effects, as well as continuous changes. The second level identifies major bottlenecks and near-bottlenecks. The third level provides a strategy for debottlenecking by considering changes in operating conditions, transferring bottlenecks from expensive to less-expensive equipment, and making structural changes. The optimization provides an investment strategy for the short, medium and long term.

c) Optimal scheduling, design, and operation of batch processes

The technology for the scheduling and planning of batch operations should, in general, take account of many issues in the supply chain. These include: the supply of raw materials, through to the process units to be used in the manufacturing, the storage and packaging operations, the transportation systems used for delivery of the products and the delivery schedules for the customers. A novel method has been developed to solve such problems (31). It uses system information and unique representations that exploit the process logistics, resulting in dramatic improvements in the potential of the mathematical methods. It is capable of providing rapid solutions, where conventional technology completely fails.

d) Operability of cogeneration and site utility systems

Variation in operation is the “norm” for many processes. Such variations may be the result of a different feed, change in the operating conditions, decrease or increase in throughput, shutdown of units for maintenance, etc. These variations will create fluctuating demands on the utility system, which must handle these changes in a cost-effective way. The design of site utility systems can now take account of operational variations (32). Optimized maintenance schedules for the utility system can also be developed.

Applications in the real world

The challenge with research in process integration is always to ensure that it works in practice. The only way to achieve this is to follow research through to application. The applications experience then needs to feed back into the research. The Dept. of Process Integration at UMIST has achieved this via the Process Integration Research Consortium, a group of 30 major companies that sponsor the research, and work closely with the researchers on the first applications of the new technology.

The Consortium provides considerable financial and technical support for the research program, and in return, receives a number of significant benefits, including specialized software packages. As this article has tried to emphasize, process-integration technology now makes significant use of mathematical programming and optimization methods. The power of these methods is undeniable, but they are virtually impossible to apply without the use of computer software. It is worth mentioning that several Consortium member companies, such as AspenTech, Linnhoff-March, and Hyprotech, have developed commercial packages based upon the research.

The close industrial links and feedback ensure that the re-

search is practically oriented and is able to help engineers to solve real problems. This claim can be backed-up by the impressive track record of industrial applications that follows below.

Pinch analysis itself has had an enormous amount of application, with thousands of projects having been carried out all over the world. Motivations have included energy cost savings, debottlenecking for increased throughput and reduction in flue gas emissions (33). Companies, such as Shell, Exxon, BP-Amoco, Neste Oy and Mitsubishi, have reported

fuel savings of up to 25% and similar emissions reductions, worth millions of dollars per year. El-Halwagi and Spriggs (6) list some industrial mass-integration applications. Here, we will look at how some of the state-of-the-art technologies discussed in this article are being applied.

The distillation-design work has seen successful industrial applications by consortium members. The dividing-wall column technology was recently applied to BP-Amoco's Coryton refinery in the U.K. The modification doubled the capaci-

Literature Cited

1. Mehta, V. and A. Kokossis, "New Generation Tools for Multiphase Reaction Systems: A Validated Systematic Methodology for Novelty and Design Automation," *Computers & Chem. Eng.*, **22**, Suppl., pp. S119-S126 (1998).
2. Mehta, V. and A. Kokossis, "A Systematic Framework for Development of Novel Multiphase Reactor Designs," presented at IChemE Research Event, Newcastle (April 1998).
3. Linke, P., et al., "Synthesis of Reaction/Separation Systems Using a Systematic Approach," presented at AIChE Spring Meeting, Houston (March 1999).
4. Linke, P., et al., "A Novel Approach for Synthesis of Reactive Distillation Systems," presented at AIChE Spring Meeting, Houston (March 1999).
5. Marcoulaki, E. and A. Kokossis, "Molecular Design Synthesis Using Stochastic Optimisation for Scoping and Screening," *Computers & Chem. Eng.*, **22**, Suppl., pp. S11-S18 (1998).
6. El-Halwagi, M. and H. Spriggs, "Solve Design Puzzles with Mass Integration," *Chem. Eng. Progress*, **94** (8), pp. 25-44 (Aug. 1998).
7. Hallale, N. and D. Fraser, "Optimum Design of Mass Exchange Networks Using Pinch Technology," *Computers & Chem. Eng.*, **23**, Suppl., pp. S165-S168 (1999).
8. Alves, J., "Analysis and Design of Refinery Hydrogen Distribution Systems," PhD Thesis, UMIST (1999).
9. Hallale, N. and F. Liu, "Efficient Refinery Hydrogen Management for Clean Fuels Production," presented at the AIChE Annual Meeting, Los Angeles (2000).
10. Shah, P. and A. Kokossis, "Systematic Optimization Technology for High-Level Screening and Scoping of Complex Distillation Systems," *Computers & Chem. Eng.*, **23**, Suppl., pp. S137-S142 (1999).
11. Shah, P. and A. Kokossis, "Novel Designs for Ethylene Cold-End Separation Using Conceptual Programming Technology," *Computers & Chem. Eng.*, **23**, Suppl., pp. S895-S898 (1999).
12. Amminudin, K., "Design and Optimisation of the Dividing Wall Column," PhD Thesis, UMIST (1999).
13. Widagdo, S. and W. Seider, "Azeotropic Distillation," *AIChE J.*, **42** (1), pp. 96-130 (1996).
14. Castillo, F., et al., "Homogeneous Azeotropic Distillation (Parts I and II)," *Ind. Eng. Chem. Res.*, **30** (3), pp. 987-1008.
15. Thong, D., "Multicomponent Azeotropic Distillation Design," PhD Thesis, UMIST (2000).
16. Soares Pinto, F., "Thermodynamic Analysis of Distillation," PhD thesis, UMIST (1998).
17. Liebmann, K., "Integrated Crude Oil Distillation Design," PhD thesis, UMIST (1997).
18. Towler, G., et al., "Improved Absorber-Stripper Technology for Gas Sweetening to Ultra-Low H₂S Concentrations," presented at the Gas Processors' Association Annual Meeting, San Antonio (March 1997).
19. Makwana, Y., et al., "A Novel Approach for Retrofit and Operations Management of Existing Total Sites," *Computers and Chem. Eng.*, **22**, Suppl., pp. S793-796 (1998).
20. Zhu, X. and L. Vaideeswaran, "Recent Research Development of Process Integration in Analysis and Optimization of Energy Systems," presented at PRES '99, 2nd Conference on Process Integration, Budapest (May 1999).
21. Wu, G., "Design and Retrofit of Integrated Refrigeration Systems," PhD Thesis, UMIST (2000).
22. Zhu, X., et al., "A Method for Automated Heat Exchanger Network Synthesis Using Block Decomposition and Non-Linear Optimization," *Trans. IChemE (Part A)*, **73** (8), pp. 919-930 (1995).
23. Asante, N. and X. Zhu, "An Automated and Interactive Approach for Heat Exchanger Network Retrofit," *Trans. IChemE (Part A)*, **75**, pp. 349-360 (1997).
24. Zhu, X., et al., "Heat Transfer Enhancement for Heat Exchanger Networks Retrofit," presented at CHISA '98, 13th International Congress of Chemical and Process Engineering, Czech Republic (Aug. 1998).
25. Manninen, J. and X. Zhu, "Thermodynamic Analysis and Mathematical Optimization of Power Plants," *Computers Chem. Eng.*, **22**, Suppl., pp. S537-S544 (1998).
26. Doyle, S. and R. Smith, "Targeting Water Reuse with Multiple Contaminants," *Trans. IChemE (Part B)*, **75**, pp. 181-189 (1997).
27. Savulescu, L. and R. Smith, "Simultaneous Energy and Water Minimization," presented at AIChE Annual Meeting, Miami Beach (Nov. 1998).
28. Singh, H., et al., "Economic Achievement of Environmental Regulations in Chemical Process Industries," *Computers Chem. Eng.*, **33**, Suppl., pp. S917-S920 (1998).
29. Boccara, K. and G. Towler, "Process Economics for Commodity Chemicals (Parts I and II)," *Ind. Eng. Chem. Res.*, **36**, pp. 3727-3755 (1997).
30. Zhang, J., "Refinery Optimization and Debottlenecking," PhD Thesis, UMIST (1999).
31. Mokashi, S. and A. Kokossis, "A Tailored Graph-Based Method for the Optimal Scheduling of Product Distribution Lines," presented at the IChemE Research Event, Newcastle (Apr. 1998).
32. Mavromatis, S. and A. Kokossis, "Hardware Composites: A New Conceptual Tool for the Analysis and Optimization of Steam Turbine Networks in Chemical Process Industries (Parts I and II)," *Chem. Eng. Sci.*, **53** (7), pp. 1405-1461 (1998).
33. Linnhoff, B., "Use Pinch Analysis to Knock Down Capital Costs and Emissions," *Chem. Eng. Progress*, **90** (8), pp. 33-57 (Aug. 1994).
34. Hamilton, R. and D. Dowson, "Pinch Cleans Up," *The Chemical Engineer*, **566**, p. 21 (1994).
35. Yokomizo, Y., Mitsubishi Chemical Corp., (1996).
36. Smith, R., "State of the Art in Process Integration," presented at PRES '99, 2nd Conference on Process Integration, Budapest (May 1999).

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ty of the column and increased the middle distillate yield by 50%, with a payback of less than one year and no operating and control problems. In addition, the azeotropic-distillation techniques have been applied in several successful joint projects with other members.

Although the reactor-system-design technology is very new, it has already seen two main applications. These were both carried out jointly with UOP.

The new heat integration and utility system work has also already seen several applications. Top-level analysis has had successful applications even though it is relatively new. The low-temperature-system design has been applied to ethylene and LNG systems. The new heat-exchanger-network retrofit methods are well-established and are now included in commercial software packages. Powergen has collaborated on the application of the power-station-design technology.

The water system design methodology has met with very impressive success, with Unilever reporting reductions of 50% in freshwater demand and 65% in wastewater production (34).

The newest member of the pinch family, hydrogen pinch, has already been taken on board by member companies, such as AspenTech, BP-Amoco, Engineers India, Exxon, ICI, Linnhoff-March, M.W. Kellogg, and UOP. Hydrogen savings experienced are typically hundreds of thousands, or even millions, of dollars per year. Alternatively, the hydrogen freed up has been used to increase partial pressures in certain reactors and enhance their conversion, yield, and selectivity, while increasing catalyst life.

Finally, Mitsubishi Chemical Corp. reports that using the new methods developed for process scheduling and supply-chain optimization, the company “can reduce delivery cost by 20-30 million Yen (about \$200,000 – \$300,000) per year” (35). These are only a few of the applications of the new technology, but hopefully they will illustrate the diversity, industrial relevance and practicality of process integration.

Challenges to wider use

Admittedly, process integration — especially the newer developments — has not been used as widely as it could be. In this author’s view, the major barrier has been simply a lack of knowledge. People will not want something if they do not know it exists! It is a pity to see that many people still think of process integration as being only related to heat-exchanger networks, as was the case in the 1970s and 1980s.

What are some of the future trends that can be expected? Robin Smith, head of Dept. of Process Integration, makes some interesting predictions (36). The first relates to the philosophy of targeting before design. Current methods still attempt, where possible, to use a two-step approach to design. First, performance targets are set to scope and screen options. Then, once the important options have been screened, a design method is used to achieve the targets. In the future, it seems probable that the boundary between targets and design will be blurred and that these will be based on more structural information regarding the process network.

Second, it is likely that we will see a much wider range of applications of process integration. There is still much work to be carried out in the area of separation, not only in complex distillation systems, but also in mixed types of separation systems. This includes processes involving solids, such as flotation and crystallization. The use of process integration techniques for reactor design has seen rapid progress, but is still in its early stages. Further work on simultaneous reaction and separation is needed. Process integration will be increasingly applied to process operations. Safety and control have still to be adequately addressed. Also, we should also not lose sight of the work still left to do in energy efficiency and emissions reduction.

Third, a new generation of software tools is expected. The emergence of commercial software for process integration is fundamental to its wider application in process design. Whilst simulation tools are now becoming quite mature and well developed, process integration software is, by comparison, in its infancy. Developments in software leading to so-called open architecture will allow process-integration software to interact online with simulation software to access physical property data and simulation models. This will make a wider range of models available to process-integration algorithms.

Ultimately, we would like to break away from having to decompose a process design into layers, and to develop an approach that treats the problem in its entirety. If we consider the rate at which process integration research is progressing, as well as the great advances being made in computer power, this vision should be a reality in the future.

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