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Process Synthesis: Design for Improved Effectiveness

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This paper sets out the motivation for using process synthesis techniques that have been developed over the past 25 years. These techniques enable developing countries to design processes that bypass the incremental improvement route. The most developed aspects of process synthesis will be discussed with particular focus on pinch technology. The technology gives emphases on both energy and capital cost targets for heat exchanger networks (HENs) and on the design techniques developed to meet these targets. A retrofit path can be identified and costed to improve on an existing process, and yield a design target to meet specified investment limits. These techniques have been applied for use in mass exchange networks (MENs), water optimization, hydrogen and oxygen usage, and production scheduling. One of the most significant developments in these areas has been the impact diagram, which shows reduction in environmental impact versus investment. Use of these techniques will lead to processes that are more effective in their use of resources and are, therefore, more sustainable.

Keywords: Energy using targets, grand composite curve (GCC), heat exchanger network (HEN), heuristics, mass exchange network (MENS) synthesis, pinch technology, process synthesis, *and* retrofit solution.

INTRODUCTION

Chemical engineering was born when it was realized that behind the great variety of chemical processes lay a set of common governing principles. This insight led to great strides, particularly in the design and optimization of individual unit operations, and even greater strides in terms of a more fundamental understanding of the microlevel phenomena that governing unit operation.

These improvements, however, did not affect the basic structure of processes. Historically, processes were developed by improvements made on existing designs. At the early stages in the development of a new technology, large improvements were possible, but the opportunities for improvement decreased with each successive generation of the technology.

The development of process synthesis techniques in the 1970s is, perhaps, the next great breakthrough in chemical engineering. This milestone led to step changes in the efficiency of by creating different configurations in the structure of the units that make up a process.

This paper explores the implications of these developments, particularly for developing countries, where new technologies are being developed to exploit their natural resources. It is argued that by applying these techniques, developing countries will no longer resort to the long incremental improvement route traditionally used in the past by the developed world. This will help them to go directly to the best process configuration, leading to more efficient processes and more competitive products.

Particular emphasis will be on the conceptual approach which led to what is known as pinch technology. The power of process synthesis will be demonstrated with examples drawn from this area of application. The brief overview that follows provides accessible references for those who wish to take them further.

PROCESS SYNTHESIS

Process synthesis is part of a wider domain within chemical engineering which is *Process Systems Engineering* (PSE). PSE has developed significantly over the past four decades and involves the systematic planning, design, operation and control of processes. A strong feature of most of PSE is the application of mathematical optimization techniques.

Within PSE, *process synthesis* is the systematic design of processes. It largely involves choosing the units in a process, as well as the links between them. It may be approached by using mathematical optimization or another approach based on thermodynamic analysis.

Process integration in turn is a subset of process synthesis, which particularly involves closer inter-linkages between process units. Process synthesis often involves a higher degree of integration between different sections of a process, but not always.

The earliest textbook on process synthesis is *Process Synthesis* by Rudd, Powers, and Siirola (1973). Another landmark book is *Conceptual Design of Chemical Processes* (1988) by J. M. Douglas. Today, there are a number of textbooks on chemical engineering design which incorporate the aforementioned approaches (Smith 1995, Turton et al. 1998, Seider et al. 1999).

Process synthesis kicked-off during the energy crises in the 70s. In 1973, oil prices increased from $1 to $10 per barrel, which in 1979 it increased further to $30/barrel (roughly where it still is today). This massive increase in energy costs meant that the chemical processing industry had to start reducing the energy costs in their processes.

This phenomenon led to a special attention being paid to energy optimization and, out of the pioneering work of Linnhoff and Flower (1978), the approach known as *pinch technology* was developed. As a result of the efforts put into it, Pinch Technology has advanced considerably and is probably the most developed area of process synthesis. The *User Guide* was a key development in this area (Linnhoff et al. 1982). The recent text on the subject by Shenoy (1995) is very comprehensive.

Process synthesis is much broader than simple energy optimization. It involves all aspects of the design of chemical processes, from the choice of processing units to the arrangements of these units to form the whole process. The process of choices mean that process synthesis is a combinatorial problem and that approaches are needed to reduce the number of options examined in detail.

Poor choices lead to inefficient structures. With such structures, the process reaches a level of performance that cannot be improved by optimizing of the parameters in the system alone. This deadend is what is known as a *topology trap*. Figure 1 illustrates the goal of process synthesis which is to perform structural optimization up front and avoid it at a later stage of design.

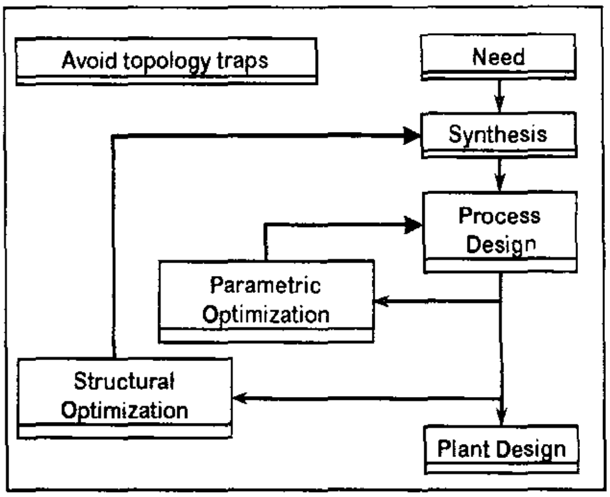

Figure 1. Goal of Process Synthesis

One approach is to break the process design into a series of steps. This approach is known as *decomposition*, or breaking the synthesis task into manageable subtasks. These subtasks are as follows (Douglas 1988):

1. *Reaction path synthesis.* Reactions are the heart of a chemical process, so any synthesis procedure needs to start here. Reaction path synthesis seeks to identify the best sequence of reactions that will help you choose the best feed and take you from there to the desired product.
2. *Reactor–recycle structure.* The reactor–recycle structure is determined by that which is produced in the reactor and the extent of conversion in the reactor. This task establishes the destination of the reactor products (recycle of unreacted feed, products, by-products, or waste).
3. *Separation system synthesis.* Once the reactor–recycle structure has been determined, the separation tasks required need to be established next. Synthesis of the separation system involves choosing the best separation technology, and sequencing the separations.
4. *Energy recovery system synthesis.* Once the reactor and separation systems have been synthesized, the energy requirements of the process will have been determined, and the energy recovery system can then be synthesized.

These tasks are not independent of one another, and they need to be integrated. Poor decisions at one stage can affect all other stages and not just the immediate stages. Douglas (1992) has also extended the decomposition approach to waste minimization.

This mythology is the basis of the conceptual approach to process synthesis, which is in turn based on the fundamental physics and chemistry involved. One example is pinch technology, which is based on the thermodynamics of energy recovery. It is, however, also a *sequential approach*, in which system analysis is done before design is undertaken.

The other major approach to process synthesis is the ,*mathematical programming approach*. In this approach, the synthesis problem is set up as a mathematical optimization problem.

Generally, this is generally done by first setting up a superstructure which has all the possible options embeds in it. This superstructure is then reduced to the best design by optimization of the units included, the connections between them, and the operations procedure. (See, for example, Papalexandri et al. 1994.)

The aforementioned is likewise a *simultaneous approach*, in which optimization and design are done together. Thus, the mathematical formulation becomes a Mixed-Integer Non-Linear Program (MINLP), because of the choices involved and the nonlinear nature of the processes and objective functions.

MINLPs are generally solved using a software that, in fact iteratively decodes an MILP problem which sets the choices and an NLP problem which optimizes the continuous variables.

Although great strides have been made as to the range of problems which MINLP techniques can solve, it is still not possible to guarantee global optimality, and the formulation of problems into a tractable form is not trivial. Thus, efforts are currently being expended to combine the strengths of these two major approaches.

Note that developing countries generally have much higher energy intensity than developed countries, where *energy intensity* is the amount of energy consumed per unit of Gross Domestic Product. While this difference is partly due to the lower production of finished goods relative to raw materials, it highlights the greater potential to save energy in developing countries.

With this background, more on to what pinch technology has achieved as an example of what process synthesis in general can do for the design of processes.

PINCH TECHNOLOGY

Probably the most significant achievement of pinch technology was the establishment of energy usage targets for processes, based on the thermodynamics of energy transfer. Until then particular industries established their own norms for energy use, in terms of usage per ton of product produced.

Plants rated themselves against these norms and were satisfied if they achieved them. When pinch technology was come up with a way to determine targets, the norms used were revealed to be much greater than what the targets showed were possible. Thus, reductions 20% to 70% were generally identified (Linnhoff 1993).

In line with this was the subsequent development of techniques to design processes to meet these targets. This move proved significant in that it validated of the targets, which on their own are meaningless, can be achieved.

The impact of these techniques on energy usage in a typical process appears in Figure 2. The graph clearly shows that the establishment of targets in the '80s drove process designers to develop techniques to meet these goals, which were achieved in the '90s. This trend means that the diminishing returns of incremental development were overcome.

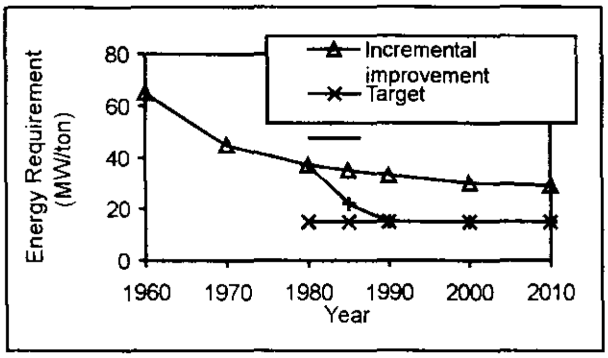

Figure 2. Impact of Synthesis

So, what does pinch technology do for the design of heat exchange networks (HENs)? Answers can be summarized as follows:

1. It provides targets for minimum energy usage (both hot utility and cold utility) and, hence, minimum operating costs;
2. It provides targets for the minimum number of exchange units;
3. It provides targets for the minimum exchange area and, hence, minimum capital costs;
4. It allows tradeoff of operating and capital costs, thereby identifying an optimum design point;
5. It provides design methods to achieve or closely approach all these targets; and,
6. Because the targets are achievable, you can compare alternative designs may be compared using targets.

Pinch technology is able to do this by looking at the energy flows in a process. Cold streams are streams that need to be heated and hot streams are streams that need to be cooled. The energy required by the cold streams is compared to the energy released by the hot streams, taking note of the temperature levels of both the energy required and the energy released, and also of the minimum driving force needed for heat transfer.

The minimum driving force for heat transfer is the *minimum approach temperature*, ΔT_{min}, which is the closest approach in temperature between a hot stream and a cold stream and, hence, between the curve representing all the hot streams and the curve representing all the cold streams.

This relationship leads to the composite curves shown in Figure 3. The point of closest approach between the hot and cold curves is the *pinch*, which is the bottleneck in energy recovery for the system concerned. Hence, the term Pinch Technology.

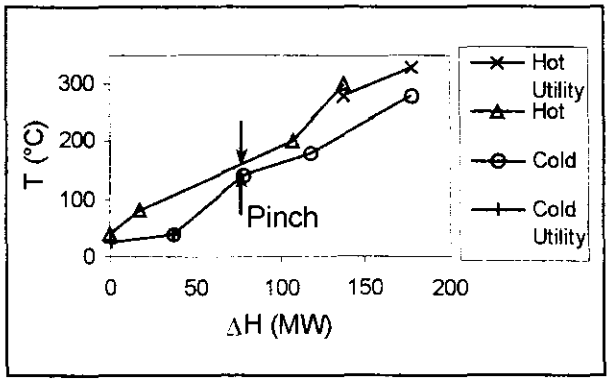

Figure 3. Composite Curves

The composite curves show the *process–process heat exchange* (the region where the hot curves and cold curves overlap) as well as the *hot-and-cold utility requirements* (the regions at the extremes where the curves do not overlap).

Note that not all processes are pinched—about 25% are not. This percentage occurs when the temperature levels of the hot and cold streams are too far apart. Such problems require only either only hot utility or only cold utility.

The composite curves also provide the basis for determining the minimum exchange area, as defined by the temperature differences between the curves, the heat transferred, and the overall heat transfer coefficients for the streams concerned, according to Equation 1.

$$A = Q / (U * T_{lm}) \tag{1}$$

As ΔT_{min} increases, the curves move further apart, leading to a higher utility requirement but with a lower exchange area. This is how energy and area are traded off, a procedure known as *supertargeting* (see Figure 4). In Figure 3, the *Total Annual Cost* (TAC) the sum of the annual utility cost and the annual capital cos.t goes through a minimum value that locates the optimum minimum approach temperature and, hence, the optimum design point for the system concerned.

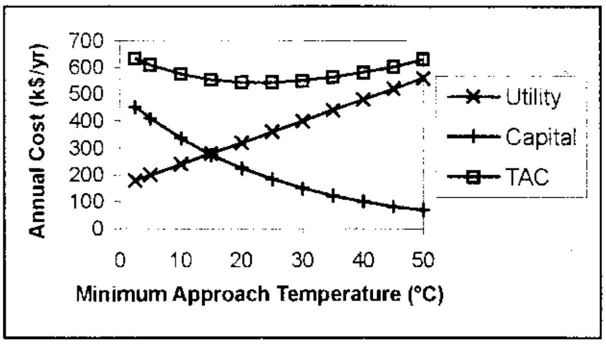

Figure 4. Supertargeting

Pinch technology also provides a means of integrating utilities in the process with the grand composite curve (GCC) shown in Figure 5. The GCC, a plot of temperature versus net energy, allows both the maximization of the *lowest cost utilities,* those closest to ambient conditions, and the generation of utilities below the pinch where this is possible. The GCC can also be used to determine the optimum levels of the utilities used for a whole site.

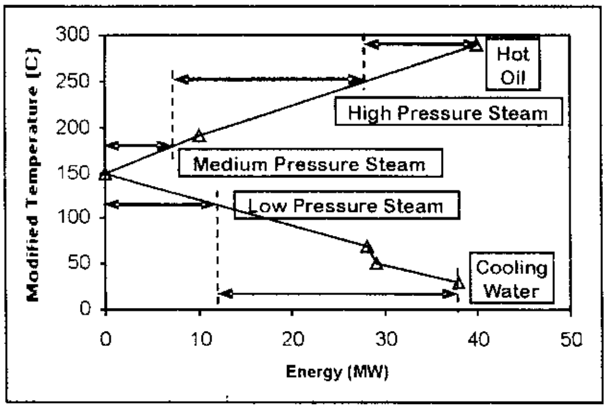

Figure 5. Grand Composite Curve (GCC)

The energy cascade in a system, as represented by the GCC, can also be used to determine the optimum location of particular items of equipment. This shows, for example, that

Can engineers system designed systems to meet these targets? While automated methods have been developed to achieve this, the *heuristic approach,* which leaves the control in the hands of the engineer, is preferred. Here, the streams are first set out on a grid diagram, such as that in Figure 6, to facilitate matching of the streams.

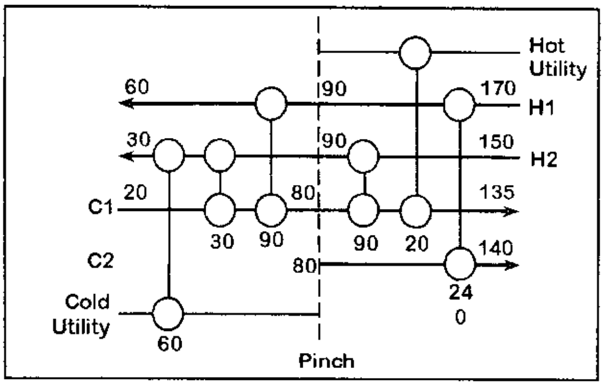

Figure 6. Grid Diagram for Stream Matching

Heuristics are rules of thumb that generally have a sound basis in experience, but cannot be proved mathematically. They guide designers in determining a good match. For matching in HENS, the following set of heuristics based on the foundation laid by Ponton and Donaldson (1974) is used:

1. Use countercurrent exchange.
2. Do not violate the minimum approach temperature. (*There are special rules for this at the pinch*).
3. Do not transfer energy across the pinch. (*This guarantees minimum energy usage*).
4. Start at pinch. (*Which is the most constrained region*).
5. Do not degrade energy. (*This can be expressed in a number of ways, such as match the hottest hot stream with the warmest cold stream and the coldest cold stream with the coolest hot stream, or avoid criss-crossing, or make best use of available driving forces*).
6. Minimize the number of exchange units. (*This tends to minimize capital costs*)
7. Consider stream splitting. (*This helps in meeting energy targets in the minimum number of units*).
8. Consider the impact of the match on what remains. *(This known as the* Remaining Problem Analysis*)*.

Application of these straightforward rules leads to designs that both meet the utility targets and closely approach the capital cost target to within 5%. The design generated in this way can also be evolved to improve the TAC.

The targets discussed above, however, are all for grassroots designs. Does pinch technology have anything to offer for retrofit situations?

Existing systems can be analyzed in the same way as grassroots systems, determining utility and area targets over a range of minimum approach temperatures. These are plotted on an Area Energy plot, and the existing system compared to the ideal curve generated by the targets, as shown in Figure 7 (Tjoe and Linnhoff 1986).

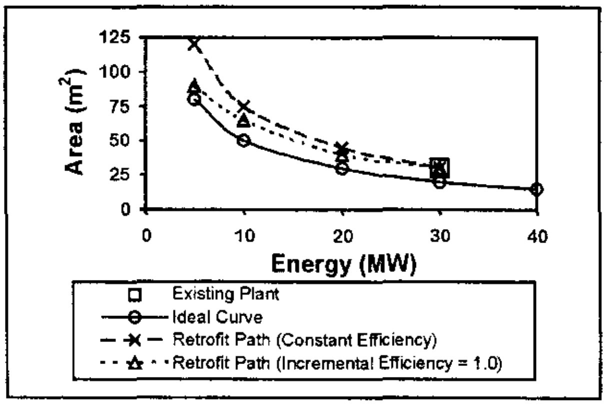

Figure 7. Retrofit Path for HENS

In retrofit, one aim is to add an extra area in order to reduce energy usage, moving to the left and upwards from the existing plant. Figure 7 shows two ways to do this: (a) by adding the extra area at the same efficiency as the existing plant, or (b) by adding the extra area at an incremental efficiency of unity. If the extra area required and the concomitant energy savings at points along the chosen retrofit path, were cast the Savings–Investment diagram shown in Figure 8 can be generated.

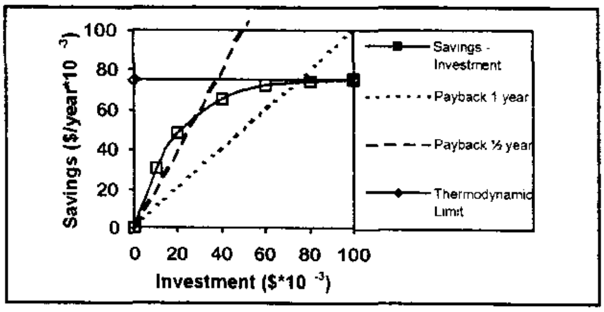

Figure 8. Savings–Investment Diagram for HENS

Retrofit studies using pinch technology have the benefit that data integrity is ensured by checking that the extra hot utility is equal to the extra cold utility. Studies we have done have found that significant savings can be achieved by making use of the following:

1. Make full use of available driving force, especially in reactor feed/effluent heat exchangers.
2. Do not cool down intermediate streams only to heat them up again.
3. Improve the operation of distillation columns. These are frequently the largest users of both heating and cooling on a plant. In many cases, columns are run at fixed reflux rates even when operating below design feed rates. Large savings are possible by simple implementing ratio control of the reflux relative to the feed. (Fraser and Gillespie 1992)

When companies require short payback times for retrofit projects, it may not be possible to justify energy savings on costs alone.

Mass Exchange Network Synthesis (MENS)

Given the well-known analogy between heat and mass transfer, it was not too long before the pinch technology approach was tried in Mass Exchanger Networks or MENs (El-Halwagi and Manousiouthakis 1989, 1990). The typical unit operations with MENs:

1. absorption and stripping (gas–liquid),
2. liquid extraction (liquid–liquid),
3. ion-exchange (liquid–solid), and
4. adsorption (gas– solid).

The variety of physical systems need different kinds of contacting devices. For these units, a Mass Separating Agent (MSA), such as water, MEA, LIX, ion-exchange resin, or activated carbon, is used to remove undesirable components from process streams.

The first target for MENS is the *utility* or *MSA target*. This is obtained by using a minimum composition difference in the lean phase, e and a composition–pickup diagram (refer to Figure 9). The line of maximum slope touching the process line represents the *minimum MSA target*.

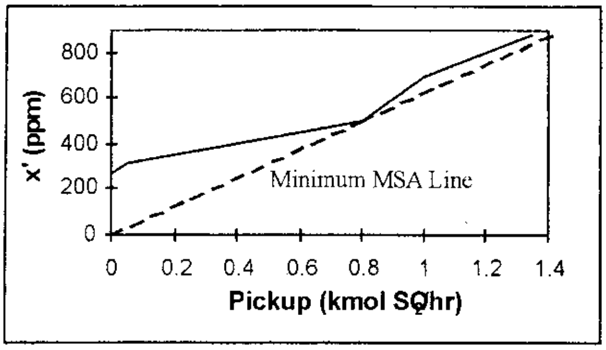

Figure 9. Concentration–Pickup Diagram

It took another ten years before the steps in formulating size targets for MENS were established. This was so because in the design of mass exchangers the driving force is not only determined by the difference in temperatures in heat exchangers, but also by the equilibrium concentration in the lean phase.

The key to this problem was the development of the *y–x composite curve plot* shown in Figure 10. This makes use of a composite operating line and an equilibrium line, targeting the size of the system of mass exchangers by stepping of the number of stages, such as on a McCabe–Thiele diagram for stagewise contactors (Hallale and Fraser 1998a, 1998b).

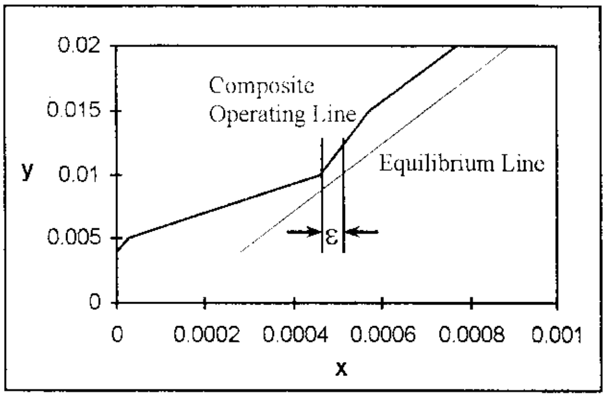

Figure 10. y–x Composite Curves for MENS

This development opened the way to perform supertargeting for MENs (Hallale and Fraser 2000b). Similarly for HENs, this is done by varying the minimum composition difference and determining the annual operating and annualized capital cost targets, leading to a diagram similar to that in Figure 4.

Methods have also been developed for the sizing of continuous contact systems and for as systems involving multiple MSAs. In the latter case, a *y–y** composite curve plot is used so that all the MSAs are brought onto a common basis by using the equilibrium concentration in the lean phase. This process also involves using a minimum composition difference in the rich phase, Dy_{min} (Hallale and Fraser 2000a).

The design of MENs follows principles similar to those in the design of HENs, such as:

1. Do not violate the minimum composition difference.
2. Do not transfer mass across the pinch.
3. Match the available driving force profile.
4. Try to minimize the number of exchange units.

Experience has shown that in mass exchange matching the driving forces are more important than minimizing the number of exchange units. The reason for this appears in Figure 11, which is the equivalent of the Driving Force Plot in HENS. Poor matches either use too much driving force or too little driving force. A match that uses too much driving force leads to a match that would have to use too little driving force. In MENS, too little driving force means a dramatic increase in size, and the operating line approaches the equilibrium line (Fraser et al. 2001b).

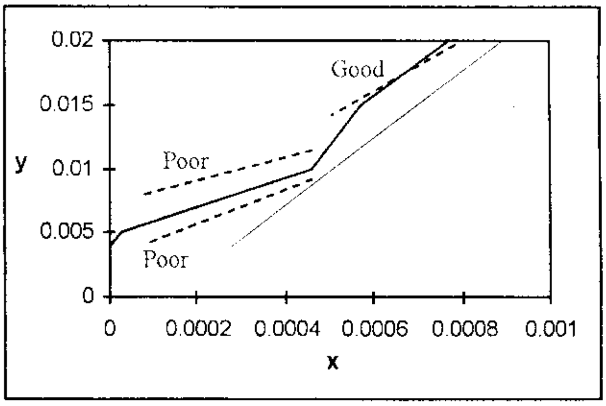

Figure 11. Driving Force Plot for MENS

It is also possible to apply the same approach to retrofit for MENS as was for HENS. In this case, a *size-load plot* replaces the *area-energy plot* (see Figure 7), and the same retrofit paths can be identified. A *Savings–Investment diagram* can also be developed, in the same way as Figure 8 for HENS (Fraser and Hallale 2000a).

In MENS, it is also possible to determine the effect of retrofit on the environmental impact of a process. For the chosen retrofit path, one can then relate the reduction in environmental impact to the investment required. This yields the *Impact diagram* shown in Figure 12. Similar to the savings–investment diagram, the graph shows a region of diminishing return on investment and the thermodynamic limit for the particular technology being used (Fraser and Hallale 2000b).

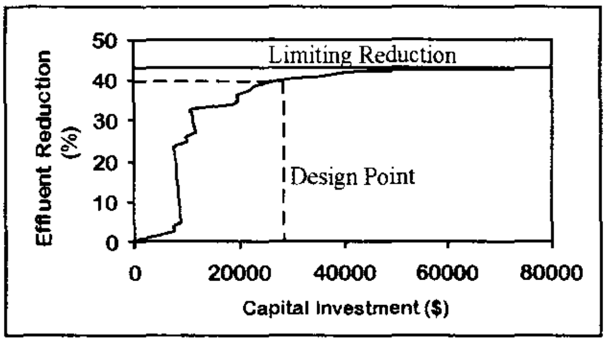

Figure 12. Impact Diagram for MENS Retrofit

The *Impact diagram* is a very powerful tool which can be utilized to determine the maximum reduction in environmental impact using a particular technology. It can also be used to compare alternative technologies, for both retrofit and grassroots designs. A *three-way tradeoff plot* has also been suggested for examining the tradeoffs among operating cost reduction, reduction in environmental impact, and capital investment.

Similar to that in HENS, the targets obtained for both grassroots and retrofit are meaningful since they can be closely approached in terms of design.

OTHER APPLICATIONS

The pinch technology approach has also been applied to a number of other uses where supply and demand are involved.

On the one hand, *water pinch* is the specific application of MENS to water usage in chemical plants, aimed particularly at minimizing the use of water (Wang and Smith 1994). On the other hand, *hydrogen pinch* has been adopted to optimize the usage of hydrogen in oil refineries. Another similar application is the *oxygen pinch*.

Beyond these three other applications is the use of pinch technology in scheduling process operations.

CONCLUSIONS

This researcher trusts that discussions on the content and scope of the applications of pinch technology will convince other researchers that process synthesis techniques will lead to:

- Early screening of design options,
- More efficient use of raw materials,
- More efficient use of utilities,
- More efficient use of capital,
- Reduction in pollution,
- Realistic pollution reduction limits, and
- More sustainable processes.

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REFERENCES

El-Halwagi, M. M. (1997). *Pollution prevention through process integration: Systematic design tool*, Academic Press, San Diego CA.

El-Halwagi, M. M., and Manousiouthakis, V. (1989). "Synthesis of mass exchange networks," *AIChe J.*, *35*, 8, 1233–44.

El-Halwagi, M. M., and Manousiouthakis, V. (1990). "Automatic synthesis of mass exchange networks with single-component targets," *Chem. Eng. Sci.*, *45*, 9, 2813–31.

Douglas, J. M. (1988). *Conceptual design of chemical processes*, McGraw-Hill, New York.

Douglas, J. M. (1992). "Process synthesis for waste minimisation," *Ind. Eng. Chem. Res.*, *31*, 238–43.

Fraser, D. M., and Gillespie, N. E. (1992). "The application of pinch technology to retrofit energy integration of an entire oil refinery," *Trans I Chem E, 70,* Part A, 395–406.

Fraser, D. M., and Hallale, N. (2000a). "Retrofit of mass exchange networks using pinch technology," *AIChEJ, 46*, 10, 2112–7.

Fraser, D. M., and Hallale, N. (2000b). "Determination of effluent reduction and capital cost targets through pinch technology," *Environmental Science and Technology, 34*, 19, 4146–51.

Fraser, D. M., Howe, A., Hugo, M., and Msiza, A. K. (2001). *Retrofit of mass exchange networks to meet cost and pollution reduction criteria,* 6th World Congress of Chemical Engineering, Melbourne, Australia.

Fraser, D. M., Hallale, N., Harding, N., Matthews, C., Jacobson, P., and Sibulela, S. (2001). *Systematic techniques for synthesis of optimum mass exchange networks,* 6th World Congress of Chemical Engineering, Melbourne, Australia.

Hallale, N., and Fraser, D. M. (1998a). "Capital cost targets for mass exchange networks. A special case: Waste minimisation," *Chem. Eng. Sc., 53,* 2, 293–13.

Hallale, N., and Fraser, D. M. (1998b). "Synthesis of a costoOptimum gas-treating process using pinch analysis," *Advances in Environmental Research, 2,* 2, 167–78.

Hallale, N., and Fraser D. M. (2000a). "Capital cost targets for mass exchange networks," Parts I–II, *Computers and Chemical Engineering, 53,* 2, 293–313.

Hallale, N., and Fraser D. M. (2000b). "Supertargeting for mass exchange networks," Parts I–II, *Trans I Chem E, 78,* Part A, 202–16.

Linnhoff, B. (1993). "Pinch analysis: A state-of-the-art overview," Part A, *Trans. IChemE, 71,* 503–22.

Linnhoff, B., and Flower, J. R. (1978). "Synthesis of heat exchanger networks," *AIChE J., 24,* 4, 633–54.

Linnhoff, B., Townsend, D. W., Boland, D., Hewitt, G. ., Thomas, B. E. A., Guy, A. R., and Marshland, R. H. (1982). "User guide on process integration for the efficient use of energy," *IChemE,* Rugby, U. K.

Papalexandri, K. P., Pistikopoulos, E. N., and Floudas, C. A. (1994). "Mass exchange networks for waste minimization: A simultaneous approach," Part A, *Trans IChemE, 72,* 279–94.

Ponton, J. W., and Donaldson, R. A. B. (1974). "A fast method for the synthesis of optimal heat exchanger networks," *Chem. Eng. Sci., 29,* 2375–77.

Rudd, D. F., Powers, G. J., and Siirola, J. J. (1973). *Process synthesis*, Prentice-Hall, Englewood Cliffs, New Jersey.

Seider, W. D., Seader, J. D., and Lewin, D. R. (1999). *Process design principles: Synthesis, analysis, and evaluation*, Wiley, New York.

Shenoy, U. V. (1995). *Heat exchanger network synthesis: Process optimization by energy and resource analysis*, Gulf Publishing Company, Houston, Texas.

Smith, R. (1995). *Chemical process design*, McGraw-Hill, New York.

Tjoe, T. N., and Linnhoff, B. (1986). "Using pinch technology for process retrofit," *Chem. Eng., 93,* 8, 47–60.

Turton, R., Bailie, R. C., Whiting, W. B., and Shaewitz, J. A. (1998). *Analysis, synthesis and design of chemical processes*, Prentice-Hall, Upper Saddle River, New Jersey.

Wang, Y., and Smith, R. (1994). "Wastewater Minimisation," *Chem. Eng. Sci., 49,* 981–1006.