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EDITORIAL NOTES

About This Issue...

By Peter R. Rony (rony@vt.edu)

With great pride, the editors present, in this issue, the 2000 Computing in Chemical Engineering award address: "Process Systems Engineering Research in the 21st Century: Some things I learned from my colleagues and mentors", by Larry T. Biegler. Larry's article is extensive - ten pages long, and we thank him for spending the time and energy to create it. It is such articles that maintain the quality and value of CAST Communications to CAST division members. Please observe that the article is copyrighted in the name of L.T. Biegler, a long-standing newsletter policy.

In this issue, we also provide, "Delivering the power of component software and open standard interfaces in Computer-Aided Process Engineering (CAPE-OPEN)", by Kerry Irons and Bertrand Braunschweig. This important article describes the CAPE-OPEN project overview and approach.

Next, we present the "CAST Policy on Technical Paper Reviews and Acceptance" policy to guide future authors and presenters at CAST-division sponsored sessions at AIChE Annual and National meetings.

As was done in the previous issue of CAST Communications, the "Meetings, Conferences, Congresses, and Workshops" section is on-line only at the CAST division web site, www.castdiv.org. This section is periodically updated more than twice a year to better serve member needs.

And About Future Issues

By Karl D. Schnelle (kschnelle@dowagro.com)

This is the second issue of *CAST Communications* that is distributed concurrently in print and on-line. The Editors and the CAST Executive Committee have been debating whether or not to take this newsletter 100% on-line through our website. Because up to 25% of our membership may miss the e-mail announcement of a new issue, we have decided not to eliminate the hardcopy. However, to reduce the time and expense of distribution, the next issue, Fall 2001, will be more of a 'hybrid": more content on-line but some hardcopy. With the Fall 2000 issue at *only* 28 pages without the Meetings section, CAST has already reduced the length of the newsletter; previous newsletters had been 40-44 pages long.

With the next issue, we will move even more content on-line. The Editors would like to test the concept by including only abstracts or the first page or two of each article in the hardcopy version. A link will be included to a webpage under www.castdiv.org, with the full text and graphics of the article. Perhaps a username/password will be used (based on your AIChE membership number). We will collect feedback and adjust subsequent issues according to CAST members' reaction to these changes. We could even in the future go to a "lower limit" of just a postcard announcement, or back to the "upper limit" of a full hardcopy version, depending on feedback received.

In either case, we will e-mail the Table of Contents and links (as soon as the on-line version has been uploaded) to everyone on the cast10 e-mail list, as well as to every AIChE CAST member who has supplied AIChE with an e-mail address. If you have any opinions or suggestions, please e-mail Peter or myself.

CAST10 E-mail List instructions are on page 22.

ARTICLES

Process Systems Engineering Research in the 21st Century: Some things I learned from my colleagues and mentors

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To start this talk, I would first like to acknowledge a number of individuals who made this award possible. I would especially like to thank my family (Lynne and Matthew), my CMU colleagues (Art Westerberg, Ignacio Grossmann, Erik Ydstie, Gary Powers and Steinar Hauan) and my CAST Colleagues (too numerous to mention here). It is also a special honor also to acknowledge my PhD advisor, the late Prof. R. R. Hughes, who was the first recipient of the Computers in Chemical Engineering Award. Finally, I am especially grateful to my best teachers: the graduate students, visitors and researchers that I have had the privilege to work with. Many thanks to all of you!

When I was notified of this award, I provided the somewhat generic title above. This title is not meant to reflect the research that needs to be done, but rather to frame some thoughts on how our research interactions and activities could be carried out. To motivate this, I thought it would be both instructive and amusing to borrow some lessons and concepts from optimization theory and algorithms. Many concepts of optimization theory have their roots in antiquity. We have all heard of the defense strategy of Queen Dido of Carthage, Heron’s behavior of the path of light and the brachistochrone problem as exercises that were conceived over two thousand years ago. Interestingly, the word ‘optimum’ was coined by Leibniz in 1710 (Beightler et al., 1979) who started with the premise:

> If God is infinitely powerful and infinitely good, then, of all possible worlds to create, He would have created only the best one – or none at all. As a result, all that happens must happen for the best.

However, Leibniz’s cheerful, fatalistic philosophy, and the hope of optimization to solve all of the world's problems, did not stand the test of time. In fact, Voltaire provided a pointed satire to this perspective through the misadventures of Candide and his mentor, Dr Pangloss - some of which cannot be repeated in polite company.

Nevertheless, the notion that Nature is optimal has remained a useful concept and was espoused by many, including Euler, Gauss, Gibbs and Hamilton, to elucidate the behavior of natural phenomena. On the other hand, while Nature seems to justify optimal behavior, it is not necessarily a good indicator of how to get there. In fact, optimization algorithms that are based on natural processes, including simulated annealing to find minimum energy states or genetic algorithms that appeal to evolution, can lead to very inefficient strategies in process engineering. For process engineering applications they are little more than *repeated case studies,* as illustrated by the interactions shown in Figure 1.

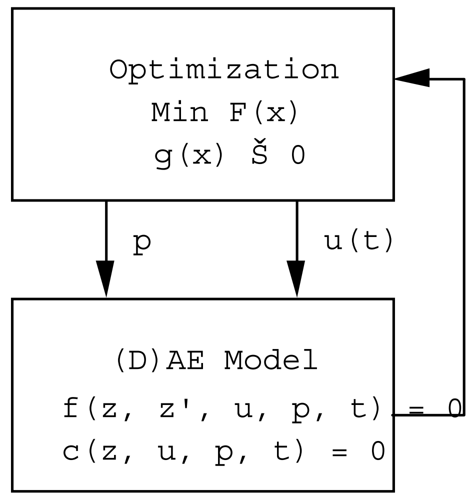


Figure 1: Repeated Case Studies?

So this leads to the first concept: how can we do things more efficiently?

Concept 1: ***Better performance is achieved when the optimum is obtained simultaneously with solution of the process model.***

I am especially grateful to Art Westerberg and Roger Sargent for teaching me this concept. Concept 1 relies on the philosophy of applying a Newton method in multivariable space. One can intuitively consider some of the variables as dependent variables that are used to solve the process model while others remain independent to guide the optimization. These are all coordinated through an optimization procedure (e.g., Successive Quadratic Programming) and the model is solved only once - at the optimum solution.

This concept was applied in process engineering by Art Westerberg over twenty years ago (Berna et al., 1980) and since then, tremendous improvements have been made in the performance of optimization algorithms. One may be tempted to think that these have been due entirely to improvements in computer hardware. To show the equal influence of optimization algorithms on performance, Figure 2 combines the effects of both by illustrating the reduction in both PC cycle time and simulation time equivalents for optimization (Biegler, et al., 2000). Note that there has been a performance increase of over four orders of magnitude in the past two decades, with over two orders of magnitude due to optimization algorithms alone.

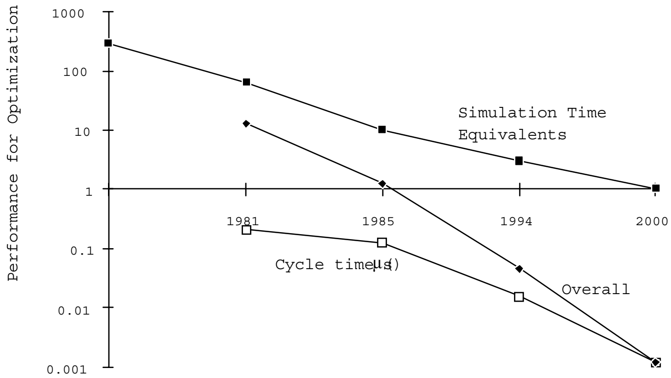


Figure 2: Effect of Simultaneous Methods on Performance

These improvements have led to a number of important practical results. In the area of *realtime optimization* (RTO), nonlinear programming strategies are applied to drive data reconciliation and model predictive control strategies. As a result, refinery setpoints and operating conditions are adjusted every few hours through large-scale problems nonlinear programs (with as many as 500,000 variables) solved with large-scale SQP algorithms. These have led to extensive applications for petrochemical processes, which have demonstrated savings of millions of dollars per year. Today, these are standard tools in refinery control and operations technology.

Similarly, the application of optimization in *process design* activities has led to

- *shorter design cycles* (with as little as 1 hr for an optimal design vs. up to 2 weeks of case studies)
- *significantly better and more consistent performance* in work processes even by less experienced engineers.,
- *better, but non-intuitive results* that arise through consideration of multiple interactions.

These activities also lead to an increased process understanding because they allow the engineer to explore the limits of process model and to get more information on process performance. As a result, lower level decisions that were made by repetitive simulation can now be handled by the optimizer, with higher level decisions handled by the process engineer, including minimum cost plants, minimum energy plants, maximum conversion cases, etc.

On the other hand, the simultaneous approach may lead to the impression that there is only one equation-solving environment that is appropriate for the implementation of Newton-type methods. In fact, these methods can be adapted to a wide variety of environments. This leads to the second concept, which was motivated initially by my PhD advisor Dick Hughes and has been reinforced by the Se-[a i]T-der brothers (Bob and Warren) and, more recently, by Omar Ghattas, a colleague in Civil Engineering at CMU.

***Concept 2:* Respect diversity**

Figure 3 illustrates three strategies for process optimization. To incorporate procedural models, and especially legacy models, into process optimization strategies, it is commonly assumed that an inefficient, nested or *modular* strategy is required. On the other hand, a fully *equation oriented* (or open form) strategy requires the reformulation of procedural models into declarative form, with the solution strategy handled entirely by the optimizer. However, if the procedural models are solved with Newton-based methods, a fully simultaneous strategy is possible, without rewriting these models. Instead, the optimization algorithm merely provides a coordination step to direct the independent variables but recognize the equal importance of the models, which are being converged internally at the same time. This tailored approach leads to the solution of much larger problems with much better performance.

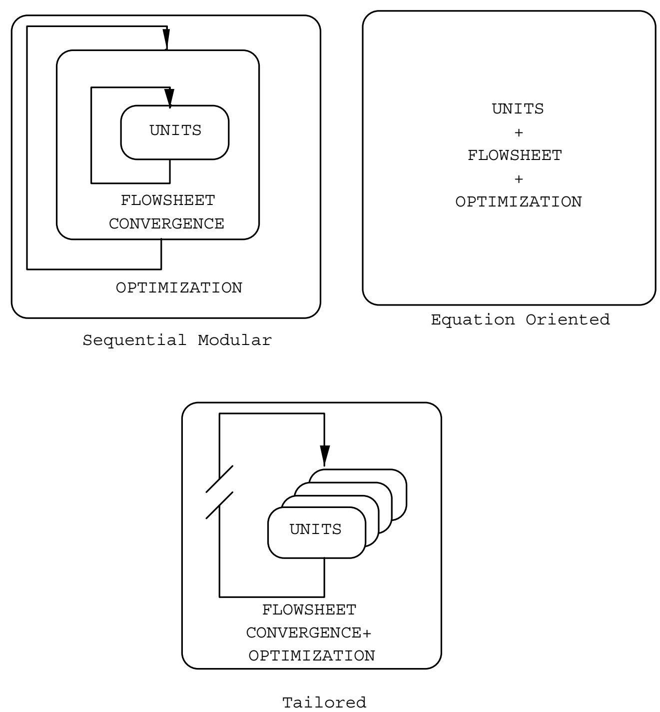


Figure 3: Different Levels of Process Optimization

To illustrate this concept, two case studies are presented next. The first is drawn from process engineering using the well-worn HDA flowsheet as the basic model. As shown in Figure 4, the flowsheet was formulated as an optimization problem originally posed by Claudia Schmid and modified by Purt Tanartkit and Dilek Alkaya. More details can be found in Biegler et al. (2000). In particular the flowsheet model contains two Newton-based procedural models, COLDAE for the reactor and UNIDIST for distillation columns. The rest of the flowsheet is modeled declaratively and the intention is to demonstrate the performance of the tailored approach. Five cases were considered where shortcut (i.e., split fraction) models are substituted by detailed Newton based models for the reactor and distillation column in the process flowsheet:

1. Product Column (UNIDIST)
2. Reactor Model (COLDAE)
3. Recycle Column (UNIDIST)
4. Both Columns (UNIDIST)
5. Reactor and Product Column (UNIDIST & COLDAE)

Here the performance of the tailored vs. the equation oriented approach is virtually identical. On the other hand, the performance of the tailored vs. the modular approach is shown in Figure 5. In each of these cases the tailored approach leads to far better performance than in the modular approach. In the last case where both models need to be considered, the tailored approach leads to a four-fold increase in performance, but without requiring open form models to be used.

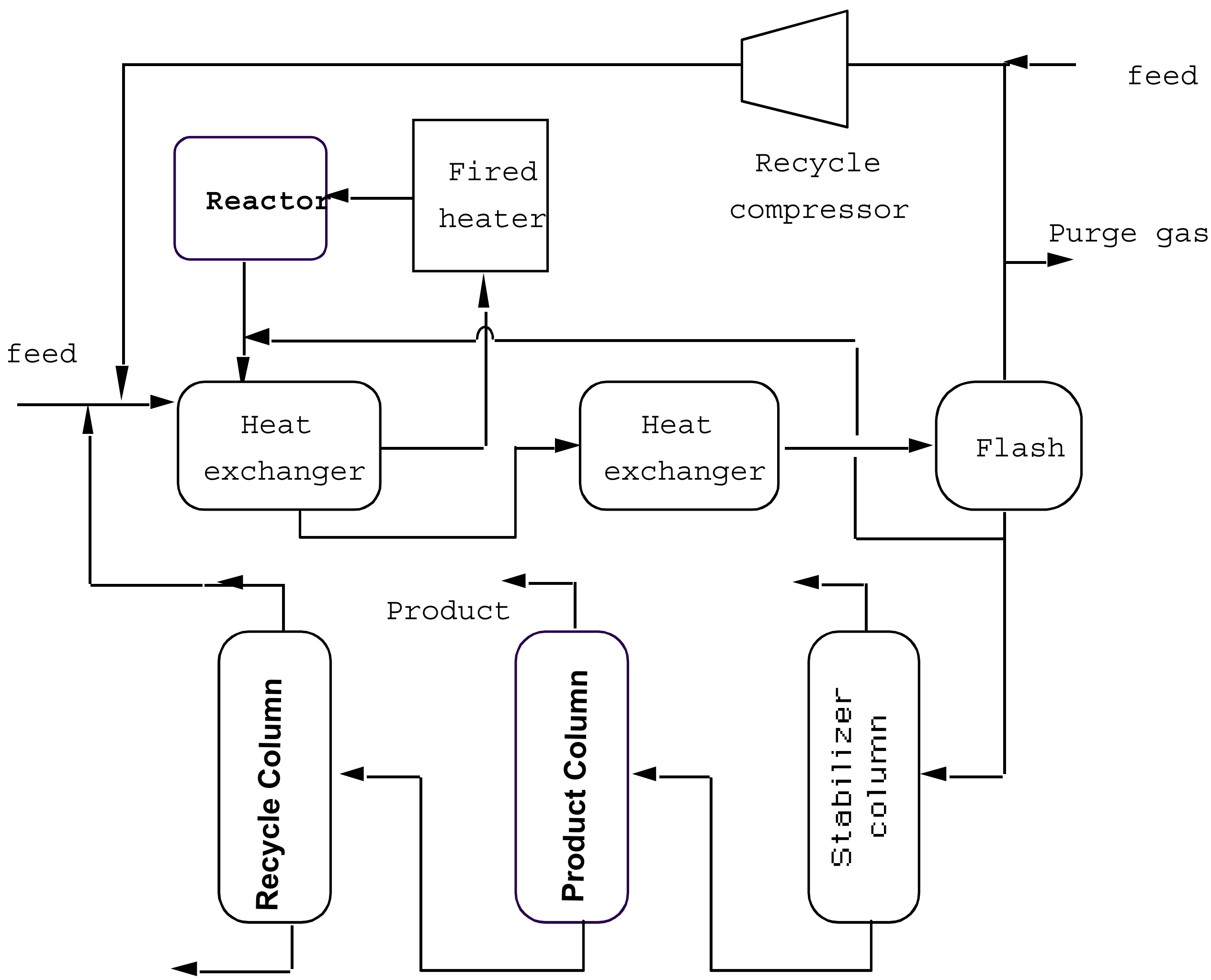


Figure 4: Modified HDA Flowsheet

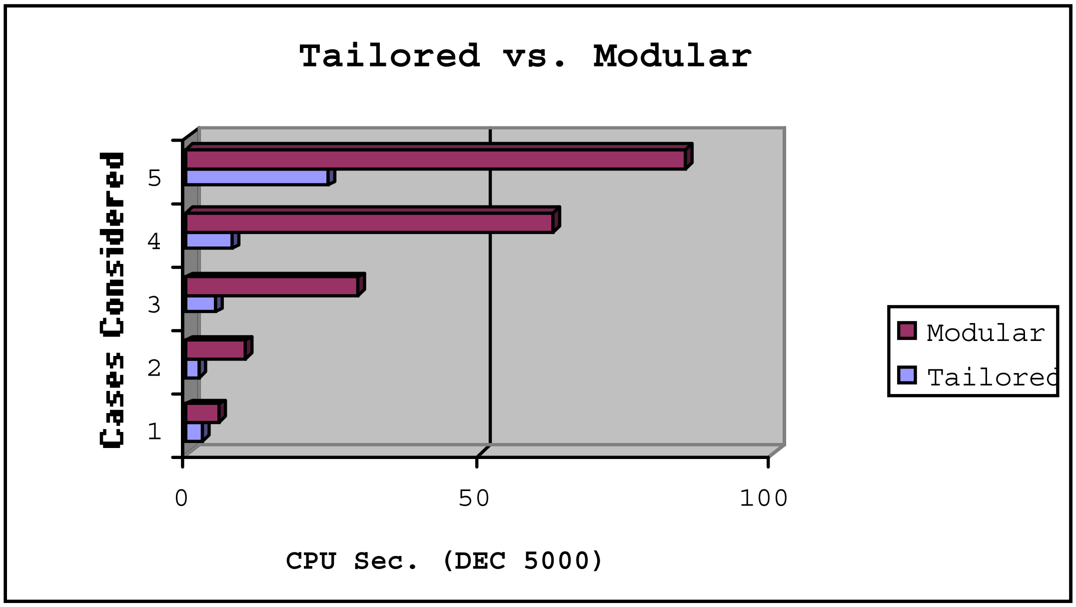


Figure 5: Comparison for HDA Optimization

In the second example, the appropriate handling of diverse structure and solvers is essential. Here Biros and Ghattas (2000) consider the active control of a three dimensional flow field around a Boeing 707 wing through fluid addition and removal. The objective is to minimize dissipation in the flow field and to solve the Navier-Stokes equations with the best control policy. The resulting discretized PDE-based optimization problem includes over 700,000 variables with 5000 degrees of freedom. To solve PDE models of this size, a Newton method is applied to the discretized equations and the resulting linear systems must be solved using preconditioned iterative solvers (e.g., conjugate gradient, GMRES). To tackle the optimization problem, Biros and Ghattas derived a simultaneous SQP decomposition strategy that makes use of these preconditioned iterative solvers directly. Their study shows that competing methods could not address this problem in any reasonable amount of time. Figure 6 illustrates the finite element approach applied for this flow field. Figures 7a and 7b present the streamlines for these flows and illustrate the fluid dissipation before and after an active optimal control strategy is applied to the wing.

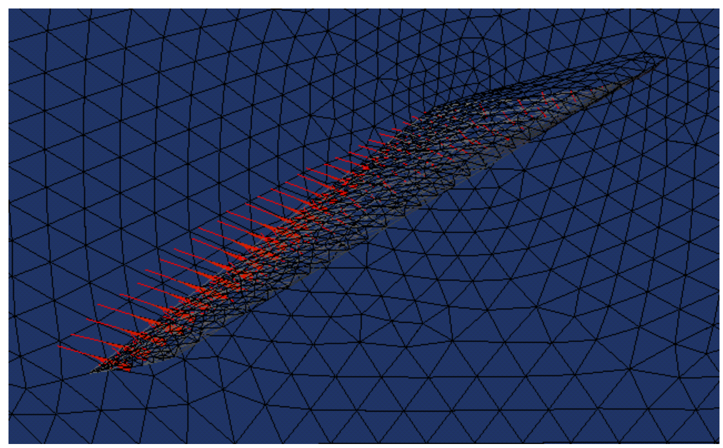
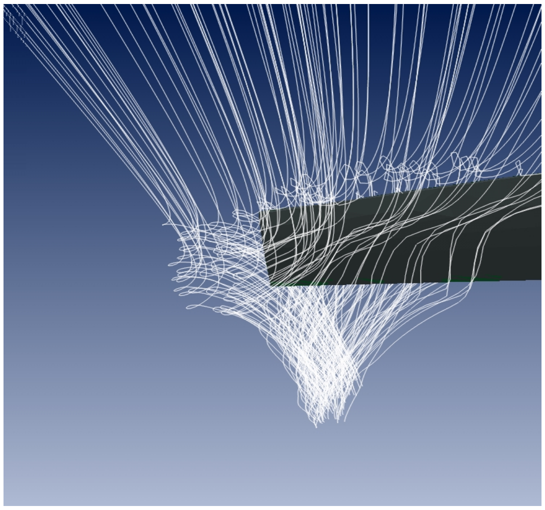


Figure 6: Finite Elements around a Boeing 707 Wing



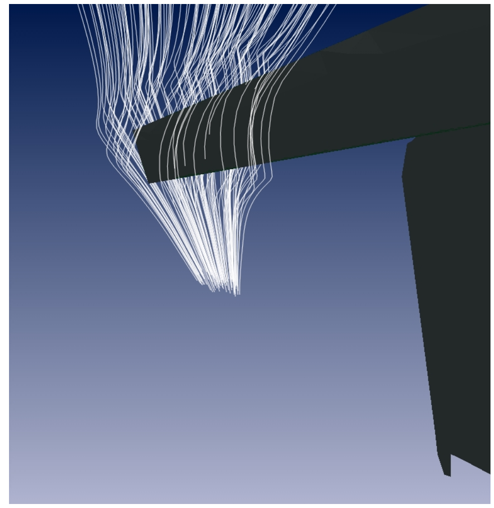


Figure 7: a) Flow with no active control, b) Flow with optimal active control

From these examples, it is clear one cannot expect these results from 'off the shelf' software where a 'one size fits all' approach is taken. Instead, these case studies show that the involvement of process engineers is essential in the development of new optimization algorithms that will be ultimately used for process engineering applications. This is in contrast to many popular views such as: *I never met a theorem I liked* or *Let the math guys do it!* Instead, as I learned from several applied mathematicians, especially Jorge Nocedal at Northwestern, attention to algorithmic details determines how methods work and how they can fail. This requires us to be especially familiar with convergence properties and the assumptions on which they are based. Moreover, as engineers we also provide the problem-based background that leads to the development of efficient calculation strategies, sensitivity analysis for ill-conditioned systems and scalability to larger systems. This attention to details also provides the key to our ownership of the research results and often makes the difference between lasting research and passing fads; it leads to the statement of the third concept:

***Concept 3*: Sweat the details to make the method work - and understand why it can fail.**

Up to this point, the focus on optimization algorithms was on performance, especially for large problems. However, if *speed* of solution is the only issue, then the benefits may not seem as interesting to practitioners, especially if most of their time is devoted to formulating the problem, not in solving it. Instead, the ability to handle larger problems more comfortably and reliably allows the engineer to step back and look at a broader problem scope. For this next concept I am grateful to Ignacio Grossmann, who pioneered and demonstrated the optimal integration of process systems on a wide array of applications:

***Concept 4:* Better solutions are obtained when systems are optimally integrated**

Over the past decade the integration of tools and process design environments has become a major activity in the process industries. The impacts of integration on standardization of work processes and incorporating design and operation issues into the supply chain (Ramage, 1998; van Schijndel and Pistikopoulos, 1999) are widely recognized as key corporate activities. Moreover, optimization is a natural tool for *integration in process engineering* as it directly handles interactions and multiple criteria. This can be seen across the board in process systems engineering (PSE). In *process design,* optimization provides the proper balance between raw material conversion, capital cost and energy consumption. In *operations,* optimization handles short term performance interactions with other processes, as well as satisfying criteria for controllability, safety and flexibility in handling uncertainty. In *planning,* optimization handles longer term interactions with other processes as well as trade-offs in demand, capacities and supplies, expansions and long range outlooks. Finally, there is an *integration among design, operation and planning*. Optimization strategies can incorporate all of these concerns (allowing them to 'talk to each other') and this has been justified with much better solutions.

Marquardt and coworkers (Helbig et al., 1998; Marquardt, 1999) demonstrated the importance of optimization tools within this integrated framework. Clearly the ability to model and optimize over entire systems and over multiple attributes leads to far superior solutions. Moreover, the integration of optimization formulations has been a fruitful activity in PSE over the past decade. Studies include integration of batch process design and scheduling (Birewar and Grossmann, 1989; Voudouris and Grossmann, 1993),