Industrial Ecology and Process Optimization

Urmila Diwekar
Mitchell J. Small
Engineering & Public Policy
Carnegie Mellon University
Pittsburgh, PA, USA

Process optimization has long been a valuable tool in chemical and product design and manufacturing.[1] Traditionally, the optimization has been structured to produce the highest quantity and/or quality of a product at the least cost, with the ultimate goal being the maximization of profitability. In recent years, environmental regulation has led to the inclusion of emission constraints as part of the optimization problem. Pollution prevention has thus moved from being a separate, add-on consideration, made only once the initial design is completed, to one that is integrated within the overall design of the product and its manufacturing process. However, industrial ecology brings the potential and perspective for the next step—where environmental considerations are not merely a constraint imposed by regulations but rather an intrinsic part of the objective function. To take this next step, where ecological considerations are fully integrated in a firm's objectives, formidable conceptual and methodological challenges must be overcome. The approach of process optimization can provide a valuable paradigm and framework for this effort.

Industrial ecology can gain significantly from the use of [process] optimization methods. These methods can be applied when constructing, validating, and calibrating models, and when solving local, regional, or global scale material and energy flow problems.

Beightler and coworkers (1967) described optimization as a three-step decision-making process, including problem formulation and system representation, determination of measures of system effectiveness, and implementation of algorithms and solution methods (i.e., mathematical procedures) to find the optimal configuration. Although much of the technical effort of process optimization focuses on the development and implementation of efficient solution algorithms, the most critical assumptions are made before this in developing the system representation and choosing the appropriate metrics for the objective function.

Problem formulation and system representation in the case of industrial ecology require the characterization of material, energy, and information flows and reservoirs, often at a combination of local, regional, and global scales. Even for a narrowly defined production process, the necessary information for the full system may be highly dispersed among various organizations and organizational units, and significant uncertainty will be present (e.g., see the analysis of a printed circuit board assembly process by Sheng and Worhach [1998]). Such problems are only multiplied when dealing with multiple firms, industrial sectors, or whole economies and multiplied again when environmental impacts are added to the equation.

For problems in industrial ecology, the second step, measuring system effectiveness, requires the inclusion of environmental considerations in the

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objective. The environmental effects of chemical releases can be estimated based on toxicity, exposure, or expected health effects, and different indices can be used to summarize these various stages of impact (again, see Sheng and Worhach (1998) for an example). However, to address issues of accuracy and the relative weighting of these indices, one must wrestle with the problem of uncertainty (e.g., Cabezas et al. 1998), in this case addressing how to value different impacts—some well characterized and some highly speculative. For example, how does one compare a highly likely impact on a localized wildlife habitat with a highly uncertain impact on human health? Environmental impacts must also be weighed and balanced against other concerns, such as cost, long-term sustainability, and employment. To further season the stew, multiple stakeholders invariably exist with different perspectives on what constitutes a good outcome. Thus, multiobjective, or multiattribute, methods are necessary to handle these different, often conflicting objectives and expectations (Cohon and Rothley 1997; Chang and Allen 1997, for a discussion of methods and applications of multiobjective optimization).

The third step in optimal design involves the development and implementation of algorithms and solution methods. The basic suite of numerical optimization techniques, including linear programming (LP), nonlinear programming (NLP), and integer programming (IP) methods, were developed circa World War II.[2] These methods have since been incorporated for chemical design in a number of large-scale process simulators.

In situations where many different plant configurations are possible and "local minima" occur,[3] advanced combinatorial methods are needed to search alternative designs in a flexible yet efficient manner. A number of creative and intriguing methods have been developed in recent years to address this need, including simulated annealing (heating and cooling of materials), which allows the optimal design to "crystallize" as an equivalent "temperature" is reduced (Painton and Diwekar 1994), and genetic algorithms, which allow the system design to "evolve" toward a fittest state, as would a species over many generations in a Darwinian environment (Reeves 1997). Other innovative methods have been developed incorporating concepts in process integration, reactor network synthesis, and optimization (AIChE Symposium Series 1994).

Although all methods mentioned above are well suited for the optimization of "static" systems, a more challenging problem is optimal control, or dynamic optimization, involving algorithms that predict time-dependent trajectories.[4] System performance is continuously monitored and assessed, and adjustments are made based both on past performance and the range of possible future inputs and perturbations. Application of optimal control demands that the system be closely followed by microprocessor-based controllers, with full computerization of the plant. As such, optimal control has only recently emerged as a feasible target for chemical and product manufacturers.

Optimal control theory can likewise provide a potentially powerful mode of analysis for global scale problems (Lempert et al. 1996). As national and global production systems and economies grow and evolve over time, system models that consider the capabilities of alternative energy technologies and the monitored response of the environment can be used to explore taxation and regulatory strategies that are both sequential and adaptive.

Whether optimization is used at the local, regional, or global level, uncertainties cannot be completely eliminated from the data or models or from the objective definition. Techniques such as chance-constrained optimization involve only minor supplements to the basic NLP or IP problem and are capable of providing useful initial insights into the behavior of uncertain systems. With chance-constrained optimization, the system is designed to perform at a particular level of reliability, no longer meeting constraints with surety but rather with a specified probability. More advanced stochastic optimization methods have also been developed to address systems with fully uncertain constraints and objectives (Birge 1997). When combined with new methods for sampling and the availability of faster computers, these allow the solution of very-large-scale real-world problems that were impossible to address in the past (see, e.g., Chaudhuri and Diwekar 1998).

In summary, industrial ecology can gain significantly from the use of optimization methods. These methods can be applied when constructing, validating, and calibrating models, and when solving local, regional, or global scale material and energy flow problems. New methods allow this to be done efficiently and with full consideration of uncertainties. We expect new applications and methodologies to continue to coevolve, each providing the motivation to address more sophisticated systems and problems. These can and should result in improved product design and production methods, and better informed industrial, economic and environmental policies.

Notes

1. For a good introduction to methods and applications, see Edgar and Himmelblau (1988).
2. The various optimization methods involve alternative techniques for searching for the best design for problems where both the system objective function and the constraints are linear (LP), the objective function and/or constraints are nonlinear (NLP), or the design space is discrete rather than continuous (IP).
3. Local minima occur when a particular design is better than all those similar (i.e., local) to it, but superior system performance can still be achieved through a major reconfiguration of the system. Many traditional NLP and IP methods can become "trapped" in such local minima and fail to identify the globally optimal solution.
4. The development of the core theory for addressing the optimization of dynamic systems actually predated, by many years, the static methods discussed above. The calculus of variations was born on June 4, 1694 when John Bernoulli posed the Brachiostochrone (Greek for "shortest time") problem and publicly challenged the mathematical world to solve it. The calculus of variations addresses problems where the decision variable is a time-dependent vector.

References

AIChE Symposium Series in Pollution Prevention via Process and Product Modifications, edited by M. El-Halwagi and D. Petrides, Vol. 90, 1994.

Beightler, C., D. Phillips, and D. Wilde. 1967. *Foundations of optimization.* Englewood Cliffs, NJ: Prentice-Hall.

Birge, J. 1997. Stochastic programming computation and applications: State of the art survey. *INFORMS Journal of Computing* 9(2): 111–132.

Cabezas, H., S. Siegel, and U. Diwekar. 1998. Evaluating impact of environmental and economic considerations on process design. Paper presented at the AIChE Spring National Meeting, New Orleans, LA.

Chang, D. and D. Allen. 1997. Minimizing chlorine use: Assessing trade-offs between cost and chlorine reduction in chemical manufacturing. *Journal of Industrial Ecology* 1(2): 111–134.

Chaudhuri, P. and U. Diwekar. 1998. Pollution prevention design. In *Encyclopedia of environment analysis and remediation*, edited by R. Meyers. New York: John Wiley & Sons, pp. 3772–3791.

Cohon, J. and K. Rothley. 1997. Multiobjective methods. In *Design and operations of civil and environmental engineering systems*, edited by C. Revelle and A. Mcrarity. New York: John Wiley.

Edgar, T. and D. Himmelblau. 1988. *Optimization of chemical processes.* New York: McGraw-Hill.

Lempert, R., M. Schlesinger, and S. Bankes. 1996. When we don't know the costs or the benefits: Adaptive strategies for abating climate change. *Climate Change* 33: 235–274.

Painton, L. and U. Diwekar. 1994. Synthesizing optimal design configurations for a Brayton cycle power plant. *Computers in Chemical Engineering* 18(5): 369–381.

Reeves, C. 1997. Genetic algorithms for the operations researcher. *INFORMS Journal of Computing* 9(1): 231–275.

Sheng, P. and P. Worhach. 1998. A process chaining approach towards product design for environment. *Journal of Industrial Ecology* 1(4): 35–55.

Address correspondence to:
Mitchell J. Small
Dept. of Civil and Environmental Engineering
CMU
Porter Hall 119
Pittsburgh, PA 15213-3890 USA
ms35@andrew.cmu.edu