Optimization of Chemical Processes, Second Edition

By Thomas F. Edgar, David M. Himmelblau, and Leon S. Lasdon, McGraw Hill, New York, 2001, 672 pp, $137.05.

This recently published work on process optimization represents an update of the original published in 1988 by the first two authors. For the second edition, Prof. Leon Lasdon has joined as coauthor and this lends the book the accessibility of optimization embedded within spreadsheeting tools like MS Excel, and Quatro Pro. Moreover, this book has a rich antecedent in the landmark text *Applied Nonlinear Programming* by Himmelblau (1967), which was one of the first books to deal with modern optimization algorithms for chemical engineering. As a result, the authors bring a rich perspective and expertise to this area. An introductory text on optimization for chemical engineers, this work brings provides a wealth of optimization algorithms and real-world applications and serves to acquaint engineers with a broad practical perspective on the subject. It is certainly a useful volume for every engineer's bookshelf.

Evolving from the previous edition, the second edition captures the evolution of process optimization research over the past 14 years. What is new in this edition are chapters on global optimization and mixed integer nonlinear programming (MINLP), as well as updated examples and methods in large-scale nonlinear programming (NLP), applications in semiconductor processing, and protein folding. Moreover, the use of the Solver tool in Excel (co-developed by the third author) has greatly extended the awareness and appreciation of optimization tools. A substantial portion of this book is devoted to its description and application.

Generally, textbooks on optimization are written from three perspectives: a rigorous mathematical treatment, numerical analysis and implementation, or an explanation for the practitioner. This text is presented solely at the third level. It provides no rigorous theorems and proofs, but relies instead on geometric and practical descriptions of properties and concepts. This approach is especially useful for an introductory text and for the practicing engineer. For advanced practitioners and researchers in this field, the absence of a more rigorous treatment will require the reliance on more mathematical texts in order to sharpen some optimization concepts, elucidate the more subtle theoretical properties and define the limits and suitability of the algorithms discussed in this text. Nevertheless, the book contains a wealth of good homework problems in Chapters 1–9, as well as an extensive list of references throughout the book. One minor point is that the authors also list supplementary references of more recent and advanced material. However, these are not cited anywhere in the text; an annotated list of these with some relevance to the corresponding chapter would have been helpful.

The text consists of three parts dealing with process optimization: formulation of optimization problems, optimization theory and methods, and chemical process optimization case studies. The text covers optimization for linear and nonlinear systems and treats problems with both continuous and discrete variables. The book does not discuss methods for the optimization with systems of differential equations, although they are referred to briefly in Chapter 14.

Part I of the text deals with problem formulation in three chapers. Chapter 1 provides a motivation for solving optimization problems and briefly discusses issues about uncertainty, scope of optimization and its impact on design and plant operations. Several examples of optimization are given (three small ones to be modeled and solved later, plus larger ones that illustrate the scope of optimization). As a motivating guideline, a general six step process for solving optimization problems is presented and illustrated with a small example. Chapter 2 provides a structure of optimization models and their development. A qualitative description is given on how to build on first principles with hierarchies of refinement. There is also an extensive description of empirical model building from data using linear and nonlinear regression. In particular, factorial designs are covered succinctly as a special case of linear least squares. Chapter 3 rounds out this part with attention paid mainly to defining an objective function in economic terms. Here, simple process examples are revisited, time value of money, and discounted cash flows are discussed along with descriptions of NPV, IRR, and payback period as desirable objectives. Parenthetically, I would have liked to see a plot of NPV vs. interest rate used as an evaluation tool; this overcomes difficulties with interpreting IRR objectives.

Part II deals with optimization theory and methods, and represents the largest and meatiest part in the book. It contains the material required to understand modern optimization methods, as well as small, illustrative examples. Chapter 4 provides concepts and geometric descriptions of nonlinear programming problems with objective and constraint contours, convexity properties for functions, level sets and feasible regions, classification of surfaces based on quadratic forms, and a qualitative derivation of unconstrained optimality conditions. Chapter 5 then deals with unconstrained optimization methods in one variable, focus on gradient and function methods in one dimension, Newton's method, regula falsi method, and quadratic and cubic interpolation methods. Fortunately, some "old chestnuts" are excluded such as the "guaranteed" golden section method. Chapter 6 discusses unconstrained optimization methods in many variables and all of the material in the previous chapter is actually repeated here. A brief description is given of random and grid search methods, conjugate direction methods, Newton's method, Marquardt's method, and trust region (TR) methods. Actually, it should have been observed that Marquardt's method is a particular TR method. It should also be noted that matrix-free conjugate gradient methods for nonlinear problems are now outperformed by limited memory quasi-Newton methods. Their treatment should replace conjugate gradients in this chapter. Finally, Chapter 7 provides a geometric description of LPs and presents a lengthy description of the simplex method (first with a numerical example, then with algebra, and then another example). Although there is a brief mention of specialized problems with network flows and assignments, there is no discussion of alternate optima (dual degeneracy) or duality in LPs and only a brief mention of more modern barrier methods. Also, it would be useful to move the presentation of quadratic programming from Chapter 8 into this chapter. Finally, the benefit of this chapter is the discussion of software with a focus on Excel for a transportation example.

Chapter 8 consists of a very long chapter on constrained nonlinear programming and takes an example based approach, without rigorous descriptions of optimization properties. To my mind, this chapter seems to cover too much material as it combines constrained methods along with available software (should use a table for this), automatic differentiation, modeling systems, and do's and don'ts for applying the software to nonlinear models. A separate chapter on some of the more software related issues would be welcome. The chapter gives a geometric treatment of the KKT conditions (without constraint qualifications), multiplier interpretations, and second-order conditions. A comprehensive list of methods is covered including quadratic programming and penalty function methods (exterior, augmented Lagrangian and barrier). SLP and PSLP with trust regions are covered at a nice level of detail, and there is a short treatment of vanilla SQP and a long treatment of GRG with motivation through numerical examples. A minor note is that MINOS is listed incorrectly among software as an SQP method. In fact, it can be described nicely in the context of a GRG method.

Two more recent topics were added to the text in this edition. Chapter 9 provides a brief treatment of mixed integer problems. Two classical integer problems (knapsack and traveling salesman) are presented along with a discussion of mixed integer linear programming (MILP) and branch and bound. Mixed integer nonlinear programming is described using a branch and bound method with NLPs, and this is illustrated on small example using the Excel Solver. Other methods including outer approximation and disjunctive programming are mentioned briefly. The chapter provides useful cautions on nonconvexity, which is the key feature in Chapter 10 on global optimization. In fact, these two chapters could be tied more closely together as an effort to overcome nonconvexities. Instead, this chapter discusses global optimization for continuous and discrete (!) problems. Methods discussed here include spatial branch and bound using αBB underestimators, multistart methods (with probabilistic properties), and heuristic methods for discrete (or discretized) problems. These include tabu search methods, simulated annealing, genetic algorithms, and an evolutionary algorithm (presented in the context of EXCEL).

Part III is devoted to applications of optimization to chemical engineering, and this sets the book apart from optimization texts. It illustrates how the methods of previous chapters are applied to chemical engineering problems and provides evidence of the richness of chemical engineering applications through these case studies. These examples are quite good, although many in Chapters 11–14 are somewhat classical. Also, Part III contains mostly small models, with an absence of network and synthesis problems (except for a case in Chapter 14), which would necessitate MILP and MINLP models. In particular, the inclusion of these problems would have provided a rich illustration of modern optimization models and algorithms. This part could also be improved by a more systematic presentation of problem formulations and statements on how they were solved (as in the CACHE GAMS Case Studies). It would also be useful to supply more information on optimization problem sizes, the performance of optimization algorithms, more information on basic modeling phenomena and modeling tips, and to make data files available on the internet so that they can be run by the reader using EXCEL, GAMS, or MATLAB.

The authors provide a useful matrix classification of optimization problem classes, as well as chemical engineering domains. Chapter 11 deals with heat transfer and energy conservation and provides simple problems related to analytical and single variable solutions, heat exchanger optimization (formally an MINLP, but solved analytically), and a linear programming power generation problem. A useful addition to this chapter would have been heat exchanger network synthesis, as it provides well studied problems for LPs, NLPs, MILPs, and MINLPs. Chapter 12 deals with useful applications for separation processes, including NLPs for distillation (the Gaminibandara and Sargent stage model), flow rate optimization with extraction column flow rates, vapor liquid equilibrium regression, and optimal reflux determination based on a shortcut model. Finally, Chapter 13 discusses fluid flow systems and begins with classical examples: an optimal pipe diameter (1-D) problem done analytically, minimum compression ratios for three stages (this could be done more generally using Lagrange functions), and a fixed-bed filter (1-D search and parametric study). Also considered is the optimal design of a gas transmission network. With fixed charges considered, this could be formulated as an MINLP, but was solved using NLP with a specialized branch and bound method.

Chapter 14 discusses reactor design and operation and presents a variety of applications. Included from the previous edition are a linear programming thermal cracker yield model, an ammonia synthesis model, and the (very old) alkylation problem. Exciting new applications in this chaper are the protein folding problem, a nonconvex unconstrained problem solved with αBB, and a low pressure chemical vapor deposition reactor. Finally, an interesting MINLP reaction synthesis problem is considered for the HDA process. The aim is to determine reactors, recycles and separators that maximize net sales. Some additional material (and even data files) would be very welcome for these examples. Chapter 15 builds on the previous chapter with the optimization of large-scale plant design and operations. Provided here are descriptions of equation oriented and modular modeling approaches with some discussion on precedence ordering, tearing, and the structure of process simulators. Examples covered include an ammonia flowsheet and hydrocarbon refrigeration.

Finally, Chapter 16 concludes the text with an interesting overview of integrated planning, scheduling, and control in the process industries. This is a timely topic and clearly demonstrates the economic benefits of the optimization strategies described in the text. Included in the chapter are the computer integrated manufacturing (CIM) hierarchy for operations, using planning, scheduling, real-time optimization (RTO), and model predictive control (MPC). This is a largely descriptive chapter that includes popular IT topics such as supply chain and ERP systems. Examples in this chapter include refinery and batch multiproduct scheduling, an MPC problem for reactor control and a small data reconciliation problem.

In summary, this is an essential text for senior level courses on chemical engineering optimization and for practicing engineers. For this audience, it is particularly enhanced by the material on the Excel Solver, which now makes optimization methods universally accessible. Moreover, to my knowledge, no other text deals with the breadth of optimization for chemical engineering. This book is a useful addition to my bookshelf and also a nice starting point for exploring new optimization topics relevant to chemical engineering.

Literature cited

Himmelblau, D. M., *Applied Nonlinear Programming*, McGraw Hill, New York (1967).

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Principles and Modern Applications of Mass Transfer Operations

By Jaime Benitez, Wiley, New York, 2002, 499 pp., $89.95.

Professor Benitez's book is a new entry into the market of textbooks intended for use in courses that teach chemical engineering separations, staged operations, and continuous contacting mass-transfer processes. Familiar texts in this group are *Separation Process Principles* (Henley and Seader, 1998), *Mass Transfer Operations* (Treybal, 1980), the pair of books by Wankat (1988, 1990), *Equilibrium Staged Separations* and *Rate Controlled Separations* and *Separations Processes* by King (1980). Of these, this new book is closest to Treybal's book in topics and approach.

Principles and Modern Applications of Mass Transfer Operations is very much focused on the traditional chemical process industries. Chapter titles are, "Fundamentals of Mass Transfer, Convective Mass Transfer, Interphase Mass Transfer Equipment for Gas-Liquid Mass-Transfer Operations, Absorption and Stripping, Distillation, and Liquid-Liquid Extraction." Each major section of the book has learning objectives, which certainly benefit the students and perhaps the instructor! A key feature of the book, which separates it from the other texts mentioned above, is the incorporation of *Mathcad* for both example problems and homework questions. A library of *Mathcad* programs for solving the Maxwell-Stefan equations, packed column calculations, sieve-tray design, binary distillation problems by McCabe-Thiele method, and multistage crosscurrent extraction is given in the appendices. These programs enable students to obtain useful solutions with less effort, as well as allow them to explore the different variables or parameters. The wide availability, low cost, and ease of use of *Mathcad* allow it to be the modern equivalent of "back of the envelope" calculations, which can be refined, if necessary, using full-scale process simulators.

The first chapter, "Fundamentals of Mass Transfer," introduces the subject formally and in significant detail covering essentially all topics of diffusive mass transfer necessary for study using this book. The author often goes beyond the standard treatment. For example, after definitions of concentration and fluxes, the Stefan-Maxwell relations are given as the fundamental model for molecular diffusion. This is a nice feature, contrasting most of the competing books, which start with Fick's Law. By starting with Stefan-Maxwell equations, such problems as chemically facilitated transport, membrane transport, (apparent) paradoxes of diffusion caused by pressure differences, and multicomponent diffusion in complex mixtures, can be described. The 17 examples in this 65 page chapter include such topics as dissolution, and effective diffusivity in a multicomponent gas mixture (related to ammonia cracking) and in a mixture of solvents. The standard problems, simple binary diffusion through a stagnant film and equimolar counterdiffusion are also included. 31 homework problems are given most with (just) the numerical answer.

The second chapter, "Convective Mass Transfer," begins by relating mass transfer in turbulent flow to the previously-solved diffusion through a stagnant film and thus defines the "F" mass-transfer coefficient in an identical fashion to Treybal (1980). Sections on dimensional analysis, and mass- and heat-transfer analogies follow (including a reprinting of Table 3.2 from Treybal comparing dimensionless groups in which we find, surprisingly, in this world of electronic publishing that the local mass-transfer coefficients k_c and k_y are copyrighted!).Through the 14 examples, 53 pages, and 26 homework problems, the author does a very good job explaining which type of mass-transfer coefficient to use for many situations and how to find a value for it.

The third chapter, "Interphase Mass Transfer," contains a very brief treatment of phase equilibria including Raoult's Law, a "modified form of" Raoult's Law (that is, activity coefficients are written for the liquid phase), Henry's Law, and K-factors for liquid-liquid systems. Given the overriding importance of phase equilibria on all of the problems in this book and all mass-transfer operations, it might have been better if a more comprehensive exposition on the topic was done. Interphase mass transfer is discussed starting with two-resistance theory; overall mass-transfer coefficients are introduced. Another couple of sections are devoted to gas side controlled and liquid side controlled situations. This is the end of the formal treatment of mass transfer and, if carefully studied, students would know rules and procedures for getting mass-transfer coefficients for a very large fraction of the situations in the process industries. However, they might have gained more understanding and ability to apply these concepts in new situations if the various coefficients and driving forces had been compared numerically and algebraically (such as to *show* that the logarithmic driving force is equivalent to a linear driving force for sufficiently dilute systems). Also, there is no discussion of mass transfer in terms of the differential transport equations; the word "boundary-layer" does not appear in the index and apparently not in the book. The rest of this chapter is a first cut at the basic procedure using mass balances and equilibrium lines for solving continuous contacting operations and equilibrium staged operations. The mass balance is used to get an operating line and the correspondence between the diagram and a real device is discussed as is the concept of minimum flow rates caused by intersection of the equilibrium and operating lines. For staged operations, the basic stepping construction is introduced. A total of 10 examples and 27 homework problems are included.

The next chapter, "Equipment for Gas-Liquid Mass Transfer Operations," describes gas-liquid packed towers extensively; bubble columns and tray columns are also included with some discussion of tray design. Enough information is given, for example, to choose packing size or, say, tray spacing, for many situations.

The title of Chapter 5 is "Absorption and Stripping". The topic is first discussed for tray columns and then for packed columns. Thermal effects are also considered for both tray and packed towers. The chapter ends with an elaborate solution that takes 8 pages for adiabatic ammonia absorption in a packed tower. 26 homework problems are included.

"Distillation" is the topic of the sixth chapter starting with flash, which is followed by simple distillation (but only for a single stage, which must leave students wondering why anyone would use it). Next comes the McCabe-Thiele method, which is covered extensively including using it with the Kremser method to deal with a large number of trays. Also, a *Mathcad* program is supplied for solving McCabe-Thiele distillation. The Ponchon-Savarit Method is not included. The chapter continues with packed column distillation, and the use of the Fenske, Underwood, Gilliland method for (approximate) calculation of multicomponent distillation,