LETTERS TO THE EDITOR

LETTER TO THE EDITOR: HANDLING OF EQUALITY CONSTRAINTS IN OPTIMIZATION

In a recent paper Westerberg and Debrosse (1973) presented an optimization algorithm which appears to suffer from the difficulty of being unable to handle nonlinear equality constraints without introducing significant errors. The optimization of an alkylation plant as described by Sauer et al. (1964) illustrates the problem at hand.

The model of alkylation plant as presented by Sauer et al. is described by 10 variables subjected to 7 equality constraints and 20 inequality constraints. In the optimization of this plant Westerberg and Debrosse have replaced 4 of the equality constraints by 8 inequality constraints so that the problem would fit into their proposed optimization algorithm. In so doing, they have allowed in essence these 4 equality constraints to be violated, and have thus increased the yield, the motor octane number, and the performance number and decreased the acid dilution factor. Although 1% change in these variables may not appear to be much, such a change is very significant. Since the estimate of the daily profit is calculated from the excess of returns over costs and these are of the same order of magnitude, such constraint violations have the effect of increasing the expected daily profit from the optimal value of $1162 to $1715, an increase of 47%. Although Sauer et al. (1964) used approximations to solve this problem by linear programming, their approximations were very reasonable, yielding an expected optimal daily profit of $1163. Also, their results were very close to the optimum values: $x_1 = 1728.37$, $x_2 = 16000$, $x_3 = 98.184$, $x_4 = 3056.05$, $x_5 = 2000$, $x_6 = 90.626$, $x_7 = 94.19$, $x_8 = 10.41$, $x_9 = 2.614$, $x_{10} = 149.58$.

With a simple modification, the procedure of Westerberg and Debrosse (1973) can be used to obtain the answer without undue approximations simply by running the problem twice. The first time the problem can be run with the approximations. Then after identifying the tight inequalities which approximate equalities, the problem can be rerun with the removal of the 1% approximations.

LITERATURE CITED

Sauer, R. N., A. R. Colville, and C. W. Burwick, "Computer Points in the Way to More Profits," *Hydrocarbon Processing Petrol. Refiner*, 43, No. 2, 84 (1964).

Westerberg, A. W., and C. J. Debrosse, "An Optimization Algorithm for Structured Design Systems," *AIChE J.*, 19, 335 (1973).

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REPLY TO LUUS' LETTER

It is unfortunate that Dr. Luus has misunderstood our use of the Sauer example. Dr. Luus attributes our replacing of the nonlinear equality constraints in the original Sauer formulation to our inability to handle them directly. This is incorrect.

To counter his interpretation, we have re-solved the original Sauer problem directly, getting essentially Sauer's answer. It required only 9 function evaluations starting from the equivalent first feasible point (that is, defined by the equivalent set of tight constraints) as used in the paper. 15 function evaluations were required in the paper.

The source of our formulation, which we stated in the paper, was Bracken and McCormick's book of solved problems (1968), a convenient source of problems on which to test the suggested algorithm. They, not us, replaced the equality constraints in contention by the perturbed inequality constraints. It is unfortunate that these changes have made the problem physically unrealistic, as shown above by Dr. Luus. We certainly would not replace equality constraints by perturbed inequality constraints as a general policy. That action should almost certainly produce a problem requiring more work.

Since the algorithm requires tight inequality constraints to be used as equality constraints while moving toward a solution, deliberately using perturbed inequality constraints to replace equality constraints and solving a problem in two passes as suggested by Dr. Luus is of no value for this approach.

LITERATURE CITED

Bracken, J., and G. P. McCormick, *Selected Applications of Nonlinear Programming*, Wiley, New York (1968).

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BOOKS (*Continued from page 1086*)

tures) and molecular models. Depth of coverage was lacking, in that none of the methods was exhaustively treated, nor were constraints and limitations completely presented.

This work is outstanding in being up-to-date with the literature at the time of its printing and for its comprehensive bibliography. We were particularly impressed with its user-oriented, engineering viewpoint. Appropriately, little space was devoted to development of theory which is adequately developed elsewhere. Each chapter summarizes the assumptions made in using the molecular models of that chapter.

In the experience of the reviewers, some of the computational procedures recommended are fraught with pitfalls for those inexperienced in the use of statistical mechanics. The shortcomings of some of the calculational methods presented should be more fully discussed. In places, the nomenclature is confusing because so many different symbols are used. However, it must be conceded that the result is uniformity, even though some of the symbols used in the text do not appear in the Table of Symbols at the beginning of the book. The obsolete Greek *digamma* used for degrees of freedom would be more easily found by the reader in the English alphabet under F.

Remarkably, we found only two specific errors. First, Equation 4-39, page 125, is dimensionally inconsistent. The difficulty lies in the given definition of $P^{(N)}$, which Reed and Gubbins define as an Nth order polynomial in r, a, and b. DeRocco and Hoover, from whom Equation 4-39 is taken, define $P^{(N)}$ as an Nth order polynomial in $1/[r \pm (a + b)]$. Secondly, Figure 8-6 is upside down. Hutchinson plotted $-\phi(r)/kT$ vs. r, whereas Reed and Gubbins consistently plot $+\phi(r)/kT$ yet the figure was reproduced directly from Hutchinson.

The problems at the end of each chapter are well thought out and are reasonably representative of the material in each chapter. Also, the appendices are extremely valuable to the reader seeking more detailed discussion, and this greater detail is quite appropriately located, since the main text is a conceptual outline leading to final equations.

In general, we were well impressed with this fine effort to accomplish a Herculean task.

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