*A Course on the*

# OPTIMIZATION OF LARGE SCALE SYSTEMS

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## INTRODUCTION

THROUGHOUT HISTORY men have employed elaborate rituals to help them reach a decision. They have poured libations, sacrificed animals, read the stars, and watched the flight of birds. They have put their faith in proverbs and rules of thumb devised to take some of the guesswork out of living. Today's management of decision-making employs a new and perhaps more scientific ritual, the use of the computer. Unaided, the human mind still cannot possibly weigh the manifold complexities involved in the operation of a business enterprise, the design of a missile, the routing of traffic or the expansion of a water resources system. Accompanying the prolific capabilities of digital and hybrid computers has been a voluminous bundle of optimization techniques.

In process design, economic evaluation, control, production scheduling, quality control, maintenance and repairs, accounting procedures, and capital budgeting the analyst is frequently faced with the problem of how to optimize complex arrangements of equipment, operations, or processes. He wishes to minimize or maximize some function termed the *objective function* or revenue function representing costs, weight, throughput, or the like subject to certain constraints. This broad class of optimization problems is usually termed the nonlinear programming problem. A natural question arises as to whether such a special topic deserves a spot in the already crowded curriculum for graduate students in chemical engineering.

Very few chemical engineers who have completed the expected undergraduate mathematics requirements can use mathematics effectively in solving optimization problems. Students are aware that if you differentiate a function and set the resulting expression equal to zero you can analytically find a minimum or maximum. What they do not realize is how limited in scope this particular treatment of an optimization problem is. It will not solve problems with stationary points nor solve constrained problems which are usually the problems of interest. Furthermore, the actual process of differentiation is often so tedious that it defeats the purpose of the technique. Therefore, it is important for the prospective practitioner of engineering to understand what tools exist to resolve practical optimization problems and what the prospects are for solving such problems.

## OBJECTIVES OF THE COURSE

The course had three main objectives:

**(1) To obtain an understanding of how to properly pose nonlinear programming (optimization) problems.**
**(2) To review the existing practical methods for solving nonlinear programming problems.**
**(3) To compare and evaluate methods of solving real problems especially those arising in the chemical and petrochemical industries.**

## SCOPE OF THE COURSE

IN THE OPTIMIZATION of a real process, the parameters and/or variables are connected by physical laws (such as the conservation of mass energy) that must be incorporated in the nonlinear programming problem as equality constraints even if they are only inferred. A second group of constraints incorporates existing limits on variables or parameters that ensure their physical realizability or compatibility with the process; the second group comprises the inequality constraints. In addition, empirical expressions, and other artifices are often introduced into a process model to describe what is occurring in the real process. It is vital that the student be able to translate the physical situation into mathematical form if the optimization problem is to be properly formulated. Consequently, after a brief initial review of about one week to bring the class members up to the same level in background information, about one week was spent in writing the functions for the nonlinear programming problem from various problem statements. Appendix A is one of the simpler problems used for such translation.

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The balance of the course was devoted approximately equally to (a) unconstrained optimization and (b) constrained optimization techniques. The broadest types of problems were examined and their solution techniques discussed, excluding, however, the following special cases:

(1) variables restricted to integer values (nonlinear integer programming)
(2) constraints involving the parameter time in the form of differential equations.

It was felt that these two topics involved special considerations that could not suitably be covered in the available time of one semester.

As might be expected, none of the existing nonlinear programming algorithms has proved to be definitely superior for all nonlinear programming problems under all circumstances. After describing the algorithms, in order to evaluate them, the course first examined the question of what criteria to use in evaluation, and then the students examined the results of several comparative studies of the various algorithms.

## METHOD OF CLASS PRESENTATION

AS IS USUAL IN graduate courses, about 60% of the class sessions were devoted to lectures describing the available optimization techniques, and going over homework that was assigned to the students. In this respect the course followed the format of a typical graduate course.

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However, because of the nature of the topic, certain special features were introduced into the course which occupied the remaining 40% of the time. First, each student received a large number of computer codes, and he was asked to solve an unconstrained and a constrained problem that he selected on each of the computer codes. Thereafter each student reported his results in class, and was questioned by the remainder of the class concerning his experience with a particular programming algorithm. The instructor participated only as a moderator, and these exchanges of information among the class were not only stimulating but produced a worthwhile appraisal of the various techniques.

Both unconstrained and constrained optimization were treated in this way, in two separate series of evaluations. Because the constrained programming codes required more user effort to execute, the extent of the exchange of information was more limited.

A second phase of the course was the assignment of individual projects in lieu of a last examination. These projects consisted of

(1) modification of existing algorithms to improve the algorithm based on the experience gained by the student in the course
(2) solution of complicated industrial problems
(3) programming of new algorithms based on articles in the recent literature or based on concepts evolved by the student from his reading and class discussion.

For students who had some knowledge of programming, the amount of creative effort introduced into the assigned project was often quite substantial.

One of the benefits to the student from these two phases of the course was that he was able to take away with him a substantial amount of software and documentation pertaining to effective optimization algorithms with known characteristics. By paying only for the cost of the cards, the student was able to obtain about 15 to 20 unconstrained algorithms and 4 or 5 of the more effective constrained algorithms. Because he had used many of the programs in his class work, he would be able in the future to introduce these algorithms as subroutines into some of his other programs or use them for class work in other courses. It was this particular feature of the class that attracted many of the students into the course because, although there were other related courses being taught in other departments, the general level of applicability of the material in those other courses was quite small. Students felt that they were unable to solve real problems after having completed the other courses.

## CONCLUSIONS FROM THE COURSE

THE COURSE SERVED a definite need in emphasizing the applications of the techniques associated with large scale optimization problems. Although the student was not trained to be a practitioner, he was able to obtain a firm grasp of the techniques available to solve real optimization problems. The course enabled the student to gain a broad mastery of nonlinear programming techniques through reading and practice. Furthermore, it fitted in well with the courses on linear and nonlinear programming, dynamic programming, control theory, network flow theory, queueing theory, and the other courses required to obtain a firm foundation in management science and operations research. The role played by the student in the exchange of information between students (and the instructor) seemed to provide considerable motivation for the course as did the provision of the computer routines and documentation.

## APPENDIX A

The power consumption of a heated stirred vessel is given by the relation:

$$P = 2.63 \times 10^{-3} FsL^5 \left(\frac{n}{60}\right)^3$$

For Reynolds numbers ( a dimensionless group encorporating the speed of rotation N and the diameter of the blade L) greater than 150, relation

$$F = \left(\frac{\mu}{3750\ snL^2}\right)^{0.05}$$

and for Reynolds numbers smaller than 150,

$$F = \frac{33.3}{\left(\frac{3750\ snL^2}{\mu}\right)^{0.75}}$$

find the lowest power consumption to mix a vessel containing 6000 gallons of a fluid for which $s = 0.8$ and $\mu = 200$.

Data: Assume for simplicity a 8 inch clearance between the impeller and the tank wall. The Reynolds number is defined as

$$Re = \frac{3750\ snL^2}{\mu}$$

The cost of the tank is \$100 per pound of metal, and the wall thinkness must be at least 1/4″ up to a 6 foot height and 3/8″ for greater height. Assume capital charges per year of 0.25 of the cost of the tank and a power cost of \$0.01 per kwh. The operating hours are 600 per year.

### NOTATION

F = empirical relation
L = impeller diameter, ft.
n = impeller speed, rpm
s = specific gravity, dimensionless
$\mu$ = viscosity, lb/(ft) (hr)

## REID & MODELL (Continued from page 172)

Some relevant data are given below:
$C_p$(vapor) = 5.8 ($H_2$) ; 7.0 ($O_2$), Btu/lbmol—°R.
Assume ideal gases.

| | Saturation Temperature at 37psia, °R | Heat of Vaporization Btu/lb |
|---|---|---|
| $O_2$ | 180 | 86 |
| $H_2$ | 43.2 | 197 |

3. Our Advanced Technology Laboratory is still attempting to find ways to separate oxygen from air. One of their more recent ideas involves the trapping of oxygen with potassium oxides, i.e., $K_2O$ would be reacted with oxygen to form $K_2O_2$ and $KO_2$. Then with a pressure- or temperature-swing cycle, oxygen gas would be released. We in the Engineering Division have been asked to comment upon this scheme and to prepare a preliminary flowsheet.

The data at our disposal are a bit fragmentary. Experiments were carried out to determine the equilibrium partial pressure of oxygen over molten potassium oxides. Samples of pure $KO_2$ were placed on a MgO boat in an evacuated tube. The tube was inserted into an oven at a sufficiently high temperature that the oxide melted. The pressure of the evolved oxygen was measured after equilibrium was attained. From this pressure measurement, the tube volume, and oven temperature, the moles of oxygen evolved could be ascertained. From this value and also the original sample weight, the atomic O/K ratio of the oxide liquid could be calculated. Next, a known amount of oxygen was bled out of the system, and