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#### CONCAVE FROGR MMING FOR GASDLIVE BLENDS

#### A. S. Manne

#### 1. Introduction

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his ; aper presents a model of the economics of motor gasoline blending -- a maximizing problem subject to certain restraints. The computations of the model cannot be handled within the framework of convertions? Lagrangean multipliers. As yet, neither George Dantzig nor I have supceeded in converting the system into a linear programming setup that is short enough to be convenient for computational purposes, and which at the same time preserves the octane technology.

Euch and Tucker [7,7] have established the theorem that a solution to this type of maximizing problem is equivalent to a certain minimax saddlepoint, and at the suggestion of Harry Markowitz, the pasoline blending model was recast into the appropriate minimax form. An iterative dirital technique was then devised for solving the minimax problem.

From a rigorous mathematical standpoint, the present iterative technique is by no means satisfactory. The method deep, however, lead to solutions that should be sufficiently accurate from the standpoint of refinery managers. Convergence takes place without an inordinate amount of computing time. All calculations were performed on a mach ne that is readily available throughout the United States -- an IEW Card

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<sup>1/</sup> I should like to acknowledge by indebtedness to Harry Markowitz, Genipe Dantzig, and to David Langfield for their many contributions to this piece of research.

<sup>2/</sup> Markowitz is currently experimenting with an analogue machine minimax solution.

Programmed Calculator, Model 2. A reneral purpose floating detail setup was employed. On the first problem run off, approximately ten nours of running time were required. For the sixth problem of this type, the running time had been cut down to less than three hours.

In order to maintain a check on the solutions, the model was kept:simple enough so that it could also be solved by graphical techniques. For that reason, the model will not in itself be of interest to refinery operators. From their standpoint, nevertheless, the computations are significant. The results bring into question the validity of a number of rules-of-thumb that are current in the industry for solving this type of economic problem. A second point: the calculations give some indication of the financial improvement that may be obtained by taking account of non-linear octane blending relationships. And finally, these machine runs have served as a pilot study, preliminary to attacking problems that involve larger numbers of variables.

The material will be presented in the following sequence: octane number prediction devices; the economic model; the computational procedure; and then a discussion of the results of the six CPC runs.

#### 2. Octane number predictions

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Like most kinds of engineering work, the forecast of gamoline octane numbers is more of an art than an exact science. Refiners themselves necessarily make paper forecasts of the octane number of proposed blends, but before marketing a product they will almost inevitably take the precaution of testing the mixture in an octane rating engine.

(a) Tetraethyl lead concentration levels.

Che phase of the problem has been investigated extensively by the refining industry -- the relationship between octane numbers and the amount of tetraethyl is lead added per gallon of a particular gesoline. It has been invariably observed



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that, as the lead concentration level is increased, the octane number increases at a decreasing rate. In order to predict this relationship, there is in widespread use an ethyl blending nonogram, reproduced as Figure 1. The points obtained by testing a particular gasoline, when plotted on such charts, will generally lie along a straight line. The line labelled "1" represents three observations for a particular gasoline reported by Bogen and Nichols. The lines labelled "2" and "3" represent two more sets of observations reported by them. In order to cut down on the number of knock engine runs, it is the general practice to test one sample of clear gasoline (i.e., no TEL) and another sample of the same gasoline containing 3 ml. of the ethyl fluid. (3 ml. typically represents the maximum allowable concentration in American motor gasolines.) These tests yield two points which can be plotted on the blending paper. The octane mumbers for intermediate lead concentration levels can then be predicted by straight line interpolation.

The ethyl blending chart that is in general use -- the one put forward by Hebl, Rendel, and Carton in 1939  $\boxed{57}$  -- was itself derived from empirical observations, and not from any algebraic formula. I have found, however, that there is a three-parameter analytic expression that gives a close approximation to the results predicted by the blending chart. Where <u>t</u> represents the octane number of the leaded gasoline, and <u>x</u> represents the TEL concentration level (in ml. per gallon):

(1)  $t = a + bx + \frac{c}{1+x}$ 

For any unknown gasoline, the three parameters, a, b, and c, have to te determined. This may be accomplished readily by taking three

1/ /T, Table 2, p. 2630.7

observations of octane number for various lead levels, and solving three simultaneous linear equations. Two observations can be the experimental ones, and the third may be determined in the standard way on the ethyl blending chart. Using equation (1) in this way, approximately 20 sets of constants have been determined for actual gasolines. Testing seven lead levels in each of these 20 cases, the equation has virtually plways given a prediction that lies within <u>•</u> 0.2 octane number of the one yielded by the blending chart.

No special significance should be attached to the particular form of equation (1). It is merely a device for enabling a computing machine to perform the same calculation as a refiner with his blonding chart and his straight edge.

(b) Two-component gascline blends.

A second phase of the blending problem is more controversial than the TEL aspect. For a lead level of, say, 3 ml., and for a 50-50 mixture of two gasclines A and B, refiners frequently calculate the octane number of the blend to be the 50-50 weighted average of the octane number of gasolines A and B each with 3 ml. The weighted average appears ratisfactory for many gasolines especially when both components are of paraffinic nature. There are, however, at least two papers publicly available — one by Eastman  $[L_7]$  and the other by Bogen and Nichols  $[1_7]$  — that call into question the straight-line averaging method. Both papers indicate that as the percentage of the high octane component in a binary mixture increases (both components initially at the same TEL concentration level), the octane level of the mixture may increase at a <u>decreasing</u> rate. Geometrically, the octane number is a <u>concave</u>, monotoneincreasing function of the percentage of the high-octane component in the blend. In ordinary language, the octane number of the blend tends to exceed the weighted average of the octane number of the blend tends to exceed

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Fig. 2—Octane number versus percent of thermally cracked component in binary blend. Three TEL levels

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Bogen and Nichols are primarily concerned with three-component mixtures, and they report only five observations at each of three TEL levels for strictly binary mixtures. The set of 15 points has been plotted, and is reproduced as Figure 2. These 15 observations are the basis for constructing the present model. For each TEL concentration level shown on this chart, straight-line interpolation has been used between <u>adjacent</u> observations. In all likelihood, these straight lines also underestimate the octane number that is attainable by blending. The existing data, unfortunately, do not provide a basis for curvilinear interpolation.

At first glance, it would appear to be a trivial matter whether octane numbers were calculated by drawing straight lines between two adjacent points or between two end points of a constant-TEL line. Nevertheless, a sample calculation presented below in Section (6) indicates that the two methods lead to TEL input requirements that differ by 20\$1

#### 3. An economic model of the blending problem

It is assumed that the refiner has available fixed quantities,  $q_1$  and  $q_2$ , of two blendings stocks - of types 1 and 2, respectively. The #1 stock is the high octane, catalytic-cracked-plus-polymer gasoline, tested by Bogen and Nichols. The #2 stock is their low octane, thermally cracked gasoline. These two may be blended together in any proportions, and may be mixed with tetraethyl lead. There are two products -- 1 and 2 -- premium and regular grade pasoline, respectively. These two are to meet minimum F-1 (Research) octane number specifications of N<sub>1</sub> and N<sub>2</sub>, and they may be sold at unit prices,  $p_1$  and  $p_2$ . The cost of 1 ml. of tetra-ethyl lead is represented by  $p_3$ .

Instead of using the two blending stocks directly for producing finished gasoline, the refiner may also elect to produce a fictitious

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intermediate product - "stock 3" - by mixing together the two initial materials in 70-30 proportions. This third stock may in turn be blended into either of the two finished products. By permitting the refiner to produce this fictitious intermediate product, the model in effect permits him to interpolate between all adjacent observations on Chart 2. There are eight independent variables in the problem,  $x_i$ , defined as follows:

> (2) x<sub>11</sub> = number of gallons of stock 1 in product 1 x<sub>21</sub> = number of gallons of stock 2 in product 1 x<sub>31</sub> = number of gallons of stock 3 in product 1 x<sub>11</sub> = ...1. of tetraethyl lead per gallon of product 1 x<sub>12</sub> = number of gallons of stock 1 in product 2 x<sub>22</sub> = number of gallons of stock 2 in product 2 x<sub>32</sub> = number of gallons of stock 3 in product 2 x<sub>32</sub> = ml. of tetraethyl lead per gallon of product 2

The set of 8  $x_1$  will be indicated by the vector  $\underline{x}$ . The refinery's net gasoline realization will be termed g(x). The net realization on one gallon of product equals the selling price of that product, less the TEL cost per gallon.

(3) 
$$p(x) = (p_1 - p_3 x_{11}) (x_{11} + x_{21} + x_{31}) + (p_2 - p_3 x_{12}) (x_{12} + x_{22} + x_{32})$$

The expression for g(x) is to be maximized, subject to certain restrictions, indicated below by (L) = (7), (9), and (10). The first condition is that the  $x_i$  must not be negative:

(4) 
$$x_1 \ge 0$$
 for all 1

Next, the TEL concentration levels must not exceed 3 ml. per gallon.

(5)  $3 - x_{ij} \ge 0$  j = 1, 2

The blending schedule, i.e. the vector  $\underline{x}$ , must not call for more of the blending stocks than the quantities of them that are available. The excess quantity, if any, of blending stock 1 will be denoted by  $f_1$ , and the excess of blending stock 2 by  $f_2$ .

> (6)  $f_1(x) = q_1 - x_{11} - x_{12} - 0.7(x_{31} + x_{32}) \ge 0$ (7)  $f_2(x) = q_2 - x_{21} - x_{22} - 0.3(x_{31} + x_{32}) \ge 0$

Finally, the two gasoline products must meet the appropriate octane number specifications. To simplify the notation, a new variable is defined,  $t_{ij}$ . This variable indicates the number of octane points by which stock <u>i</u> exceeds (algebraically) the specifications for product <u>j</u>, when  $x_{ij}$  ml. of lead are added to stock <u>i</u>. The variable  $t_{ij}$  is evidently a function of  $x_{ij}$ , and is determined through the following relations

(8) 
$$t_{ij}(x_{lij}) = a_i + b_i x_{lij} + \frac{c_i}{1 + x_{lij}} - N_j$$

In order to ensure meeting octane number specifications, the following conditions must then apply:

> (9)  $f_3 = x_{11} \cdot t_{11}(x_{11}) + x_{21} \cdot t_{21}(x_{11}) + x_{31} \cdot t_{31}(x_{11}) \ge 0$ (10)  $f_4 = x_{12} \cdot t_{12}(x_{12}) + x_{22} \cdot t_{22}(x_{12}) + x_{32} \cdot t_{32}(x_{12}) \ge 0$

The mathematical problem posed here is the maximization of expression (3), subject to conditions (L)-(7), (9), and (10). Before going on to the computational procedure, it is worthwhile to reexamine some of the assumptions that have been slipped into the analysis.

Aith the exception of the octane blending relationships, these accumptions closely resemble the ones underlying the avgas linear programming model of Gnarnes, Cooper, and Mellon  $\int 2.7$ . Like the earlier model, I have accumed that the quantities of blending stocks available and that the octane characteristics of these blending stocks are independent of decisions in the blending department. In fact, from the viewpoint of a refinery superintendent, these quantities and characteristics are-variables subject to control. By altering the reactor temperatures, the recycle ratios, and the assignment of intermediate distillate oil streams, the central management is able to influence the size and composition of the gasoline blending materials This type of interlock can only be studied in a larger model that cuts across departmental lines.

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Again, like the linear programming system, the present one assumes that unlimited quantities of tetracthyl lead may be purchased at the going rate, and that unlimited quantities of premium and of regular grade gasoline may be marketed at the current spot price. Such assumptions are probably realistic for the smaller refiners, but they are open to serious doubt in the case of the major ones. For the latter, a more complex type of g(x) payoff function is certainly in order. Lacking this more complex function, I have fallen back on the simpler one. The economist can at least comfort himself with the thought that equation (3) is the one usually employed by iniividual departments within a large refining organization.

In one respect, the model at hand is less complex than the one developed by Charnes, Cooper, and Nellon. Theirs includes a maximum wapor pressure specification, as well as the minimum octane condition  $\sum 2$ , pp. 138-1417. In future work, the concave programming model will be expanded to incorporate additional restrictions of this nature. Since these other properties blend

linearly, they can be included without a large increase in the time required for computing.

#### L. The computational procedure

Kuhn and Tucker have proved the following "equivalence theorem": "Let the functions  $f_1(x)$ , . . .  $f_{\pi}(x)$ , g(x) be concave as well as differentiable for  $x \ge 0$ . Then  $x^0$  is a solution of the maximum problem if, and only if,  $x^0$  and some  $u^0$  give a solution of the saddle value problem for  $\emptyset(x,u) \equiv g(x) + u^{2}Fx$ ."

For the gasoline blending case, g(x) is given by equation (3) above, and the  $f_j(x)$  by (6), (7), (9), and (10). The reader can verify for himself that all these expressions are differentiable, and that (3), (6), and (7) are concave. Furthermore, (9) and (10) will be concave over the range  $0 \le x_{Lj} \le 3$ . In other words, if we have the answer to the problem of minimaxing  $\emptyset(x,u)$ , we also have the answer to the problem of maximizing (3), subject to restraints (b), (5), (6), (7), (9), and (10). The computational problem is that of finding a minimax for  $\emptyset(x,u)$ .

- $1/[7, p. L86_7]$  The expression u'Fx is shorthand for the following:  $u_1 f_1(x) + u_2 f_2(x) + ... + u_m f_m(x)$ . The  $u_1$  are non-negative Lagrangean multipliers, and correspond closely to the economist's notion of "shadow prices".
- 2/ Note that in the present version, there are not only lower limits on the individual  $x_1$  imposed by expression (4), but also upper limits on the  $x_{1j}$ , determined by (5). For computational purposes, it was easier to impose these upper limits, rather than to set up additional  $f_j(x)$ restrictions. The upper limits make no essential difference in the applicability of the "uhn-Tucker theorem.

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The computational procedure is an iterative one, at each step  $\underline{t}$ , converting a vector  $\mathbf{x}(t)$ ,  $\mathbf{u}(t)$  into a new vector  $\mathbf{x}(t+1)$  and  $\mathbf{u}(t+1)$ . The solutions observed have <u>tended</u> toward the minimax point, but I can give no strict proof of the necessity of this convergence.' The new vector generated is not necessarily "attainable", nor is it usually "efficient" in the sense of Koopmans  $\underline{f}(t, p, 79\underline{7})$ . "Profits" do not increase monotonically as they do at each step of Dantzig's simplex procedure for linear programming  $\underline{f}_3\underline{7}$ . Despite these apparent shortcomings, the algorithm gives useful answers in the cases examined to date.

The solution must be started off from some initial vector  $\mathbf{x}(0)$ ,  $\mathbf{u}(0)$ . In principle, this may be any arbitrary non-negative vector. In practice, though, there will be a considerable reduction in computing time if a "good" initial position is selected. At each step, first the <u>u</u> vector is determined, and then the <u>x</u> vector. For the former, the basic iteration consists of two steps, and for the latter, of four steps. The problem is one of determining  $\triangle u_j \equiv \mathbf{u}(t+1) - \mathbf{u}(t)$ , and  $\triangle \mathbf{x}_i \equiv \mathbf{x}_i(t+1) - \mathbf{x}_i(t)$ . The procedure looks cumbersome, but less than two minutes of machine time are required for generating the whole set of  $\triangle u_j$  and  $\triangle \mathbf{x}_i$ . For the  $\triangle u_j$ , the procedure is as follows:

1. If 
$$\frac{\partial \phi(t)}{\partial u_j(t)} \ge 0$$
, then the "candidate"  $\Delta u_j = -k_j$   
If  $\frac{\partial \phi(t)}{\partial u_j(t)} < 0$ , then the "candidate"  $\Delta u_j = k_j$ 

Note: kj is an arbitrary positive constant.

2. If 
$$u_j(t) + \Delta u_j < 0$$
, then  $\Delta u_j = -u_j(t)$   
If  $u_j(t) + \Delta u_j \ge 0$ , then  $\Delta u_j = \widehat{u_j}(t)$ 

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For the  $\Delta \mathbf{x}_i$ , the procedure becomes:

1. If, for any 
$$\underline{j}$$
,  $f_j(t) < 0$ , and if  $\begin{bmatrix} \frac{\partial \mathscr{J}(t)}{\partial x_i(t)} & \frac{\partial f_j(t)}{\partial x_i(t)} \end{bmatrix} < 0$ , then

 $\Delta x_1 = 0$ ; proceed to evaluate  $\Delta x_1 + 1$ . Otherwise, proceed to step 2.

2. If  $\frac{\partial \phi(t)}{\partial x_1(t)} \ge 0$ , then the "candidate"  $\Delta x_1 = k_1$ 

If 
$$\frac{\partial \beta(t)}{\partial x_1(t)} < 0$$
, then the "candidate"  $x_1 = -k_1$ 

Note: ki is an arbitrary positive constant.

- 3. If  $x_i(t) + \Delta x_i \le 0$ , then  $\Delta x_i = -x_i(t)$ ; proceed to evaluate  $x_i + 1$ . If  $x_i(t) + \Delta x_i \ge 0$ , then proceed to step 4.
- 4. If  $\underline{i} \in \mathbb{N}$ , and if  $i \in \mathbb{N}^2$ ,  $\Delta x_i = \widehat{\Delta x_i}$ ; proceed to evaluate  $x_i \in 1^+$

If  $\underline{i} = L1$ , or if  $\underline{i} = L2$ , calculate  $3 - x_{Lj}(t) - \Delta x_{Lj}$ . If this expression is non-negative,  $\Delta x_{Lj} = \overline{\Delta x_{Lj}}$ . Otherwise,  $\Delta x_{Lj} = 3 - x_{Lj}(t)$ . Proceed next to evaluate  $\Delta x_{i+1}$ .

For the  $\wedge$  u<sub>j</sub>, the explanation of this ritual is straightforward. Step (1) tells us to decrease u<sub>j</sub> by an arbitrary arount k<sub>j</sub> if, for a "small" change in u<sub>j</sub> <u>alone</u>, the effect will be to decrease  $\emptyset$ . Similarly<sub>r</sub> there is to be an increase in u<sub>j</sub> if, for *e* "small" increase,  $\beta$  would decrease. Step (2) prevents u<sub>j</sub> from becoming negative. For the A x<sub>i</sub>, the justification is more tortuous. (Steps (3) and (4) are the obvious ones - respectively, lower and upper limits on the individual x<sub>i</sub>.) As with the A u<sub>j</sub>, the sign of  $\frac{\partial}{\partial \frac{\beta}{x_i}} \frac{(t)}{(t)}$  is primarily the criterion that determines whether to take a positive or a negative step. Preliminary hand calculations indicated, however, that the unqualified "direction of ascent (descent) rule" would lead to major oscillations during the process of convergence. For that reason, rule (1) -- a relaxationtype principle -- was inserted. Translated into English, the statement reads, "If one of the restraints is being violated, and if the directionof-ascent rule would lead to an even greater violation of this restraint, then the particular x<sub>i</sub> should not be changed." An IBM run is now in process for purposes of comparing the efficiency of the relaxation-type algorithm with that of the urmodified direction-of-ascent operation.

- 1/ The reader should note that  $\emptyset$  is being minimized with respect to  $\underline{u}$ , and maximized with respect to  $\mathbf{x}$ .
- 2/ Since the original draft of this manuscript, the run has been completed. At the end of 110 steps, there was still no evidence of convergence.

Parameter values and initial conditions were identical with those for run 6. The only difference was the elimination of step (1) for the computation of  $\wedge x_1$ . For the reader's convenience, the time series on three of the variables are indicated below:

$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	t	x <sub>31</sub> (t)	$x_{22}(t)$	$u_{l}(t)$
10 $1,368.6$ $651.4$ $11.90$ $20$ $1,128.6$ $451.4$ $11.50$ $30$ $1,128.6$ $611.4$ $11.90$ $10$ $1,128.6$ $531.4$ $11.90$ $50$ $1,308.6$ $651.4$ $11.50$ $60$ $1,185.6$ $651.4$ $11.90$ $70$ $1,216.6$ $491.4$ $11.30$ $80$ $1,308.6$ $651.4$ $12.30$ $90$ $1,048.6$ $531.4$ $11.70$ $100$ $1,308.6$ $731.4$ $11.70$ $110$ $1,068.6$ $651.4$ $11.70$	0	1,428.6	571.4	12.10
201,128.6 $151.1$ 11.50 $30$ 1,128.6 $611.1$ $11.90$ $10$ 1,128.6 $531.1$ $11.90$ $50$ 1,308.6 $651.1$ $11.50$ $60$ 1,185.6 $651.1$ $11.90$ $70$ 1,218.6 $191.1$ $11.30$ $80$ 1,308.6 $651.1$ $12.30$ $90$ 1,008.6 $531.1$ $11.70$ $100$ 1,308.6 $731.1$ $11.70$ $110$ 1,068.6 $651.1$ $11.70$	10	1,368.6	651.4	11.90
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	20	1,128.6	151.4	11.50
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	30	1,1,28.6	611.4	11.90
501,308.6 $651.4$ $11.50$ $60$ 1,155.6 $651.4$ $11.90$ $70$ 1,218.6 $191.4$ $11.30$ $80$ 1,308.6 $651.4$ $12.30$ $90$ 1,008.6 $531.4$ $11.70$ $100$ 1,308.6 $731.4$ $11.70$ $110$ 1,068.6 $651.4$ $11.70$	LO	1,128.6	531.4	11.90
601,155.6 $651.h$ $11.90$ $70$ 1,218.6191.4 $11.30$ $80$ 1,308.6 $651.h$ $12.30$ $90$ 1,008.6 $531.4$ $11.70$ $100$ 1,308.6 $731.4$ $11.70$ $110$ 1,068.6 $651.4$ $11.70$	50	1,308.6	651.4	11.50
701,248.6491.411.30 $80$ 1,308.6651.412.30 $90$ 1,008.6531.411.70 $100$ 1,308.6731.411.70 $110$ 1,068.6651.411.70	60	1,185.6	651.1	11.90
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	70	1,216.6	491.4	11.30
90 1,008.6 531.4 11.70   100 1,308.6 731.4 11.70   110 1,068.6 651.4 11.70	80	1,309.6	651.li	12.30
100 1,308.6 731.4 11.70   110 1,068.6 651.4 11.70	90	1.0.8.6	531.4	11.70
110 1,068.6 651.L 11.70	100	1, 308.6	731.4	11.70
	110	1,068.6	651.L	11.70

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Run Number		1	2	3	4	5	6
	St: ps 1-119	Steps 150-346					
F1	12.00	12.00	12.00	12.00	12.00	11.60	12.00
P3	0.23	0.23	0.23	0.23	0.23	0.23	0.60
41	1,000.	1,000.	1,000.	500.	300.	1,000.	1,.00.
F = 1	LO.	10.	. i.b.	20.	20.	201	10
	10.	20.	20.	20.	20.	<u>20</u> .	20.
; •1	56.	56.	0	30.	20.	30.	30.
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41.2	J.12	J. E	0.96	د <b>ر.</b> د	0.03	0.03	U.03
k <sub>3</sub>	0.60	<b>১.1</b> র	0.15	0.10	0.10	0.10	0.10
lk <sub>2</sub> ∣	0.13	J <b>.1</b> 5	0.15	0.10	J <b>.1</b> J	5.10	J.10
F.	0.000	0.003	S-1-2	J.223	0.001	0.003	ം.ധ3
kL	0.006	0.003	Q	0.003	0.003	0.013	0.003

Table 1. Parameters for Six Sets of Calculations

At the present time, I am in an unpleasant quandary concerning the logic of these computational techniques. On the one hand, I have been unable to prove the necessity of convergence for either the modified or the unmodified procedure. On the other, I have been unable to construct a counter-example for a case where the  $k_1$  and the  $k_j$  may be made arbitrarily small. Even worse, there is not yet any general criterion for determining whether the relaxation-type procedure increases or decreases the efficiency in computing out a particular numerical example. These are all problems on which I will welcome mathematical advice.

#### 5. Six computation runs

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During the course of six IBM runs, the only numerical parameters altered were:  $p_1$ ,  $p_3$ ,  $q_1$ , the  $k_1$  and the  $k_3$ . The individual values for these are listed below in Table 1. The remainder were maintained at the values indicated in Appendix I.

In order to provide the most severe test of the computational procedure, the first run was made with a distinctly non-optimal initial position — in fact, from the zero vector for all  $x_i$ . (Exact numerical values for the x(0) and u(0) of each run are listed in Appendix II.) This non-optimal feature shows up in the time series for the first 20 steps (Figures 3-7). Most of the  $x_i$  indicate a strong upward trend during this initial phase. The only legitimate inference that can be drawn from the series at step (20) is that nothing like a stationary equilibrium has been reached. In fact, there continued to be significant trends in the  $x_i$  until 200-300 iterations had been performed. The process was finally stopped at the 3h6th step. The meries for steps 327-3h6 are reproduced as Figures 8-12, and the vector at this point is given in Column A of Table 2.

Even at the 316th step, the system is not at a saddle point. According to the graphical solution (column C), at the optimum point  $x_{11} = x_{12} =$  $x_{22} = x_{32} = 0$ . Although the IBM tabulation does indicate zero levels for  $x_{12}$  and  $x_{32}$ , nevertheless,  $x_{11}$  and  $x_{22}$  both show up at low positive levels.

More serious, the exact solution is infeasible. For example, the schedule requires more of stock 2 than is available -- 1,026.h gallons, as against the 1,000 gallon limit. Only a simple adjustment is required, though, in order to obtain feasibility. The entries for  $x_{11}$ ,  $x_{21}$ ,  $x_{31}$ , and  $x_{22}$  were each multiplied by  $\frac{1,000.0}{1,025.4} = 0.97h28$ . In order to satisfy f<sub>3</sub>, it was necessary to make a slight increase in  $x_{h13}$  f<sub>h</sub> could be satisfied with a lower value of  $x_{h2}$ . Finally, it was noted that the adjuctment to the  $x_1$  left h3.6 gallons of stock 1 in excess. Since stock 1 can be sold as premium grade gafoline by adding only 0.80 ml. of lend, this h3.6 gallon excess was credited to profits af a value of ll.816  $\frac{1}{2}$ /gallon. The adjusted blending schedule is both feasible and efficient. The payoff, g(x), amounts to \$230.58 as against a possible \$231.03, indicated by the graphical solution. These two numbers coincide to within 1 part in 500 -- well within the limits of accuracy of the graphical method.

Having established the general convergent nature of the algorithm, the remaining calculations were carried out from initial vectors that were coneidered to be sensible starting points. Run 2 was started off from C., the vector that is labelled "graphical solution" in Table 2. The solution never departed markedly from the initial values, and was halted at the 63rd step, giving a second column labelled "A., raw vector" in Table 2. The rough solution was adjusted in the same way as has been described for run 1, and the results also entered in Table 2. The adjusted g(x) = -3228.62 = - is again acceptably close to that for the graphical solution,  $\frac{1223.73}{2}$ .

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Fig. 10-Final 20 steps of run number 1



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Fig. 11—Final 20 steps of run number 1



Fig. 12-Final 20 steps of run number 1

	Run 1			Run 2		
	A. Kaw Vector	B. Adjusted Vector	C. Craphic Solution	A. Raw Vector	B. Adjust∺d Vector	C. Graphic Solution
Final t	346			63		
<b>x</b> 11	80	77.0	υ	960	960	1,000
x <sub>21</sub>	560	515.6	571.4	n20	920	1,000
× 1	1,299	1,254.9	1,429.6	0	0	J
x <sub>ll</sub>	1.92	1.95	1.95	2.38	2.40	2.45
×12	0	0	0	a	0	0
×22	80	77.9	0	80	80	0
x <sub>30</sub>	υ	υ	о	0	0	Ö
x <sub>1.2</sub>	0.72	0.70	0	0.8L	0.70	U
f <sub>1</sub> (x)		43.6			F2.0	
$f_{\hat{c}}(x)$		υ			J	
g(x) (Bollar	y) 231.51	2.0.2g	231.03	223.95	228.62	228.73

	Run 3			Run L		
	A Raw Vector	<u>B</u> Adjusted Vector	<u>C</u> Gruphic Solution	A HEW Vector	B Adjusted Vector	Cr.this Cr.this Clution
Final t	70			30		
<b>x</b> 11	0	0	Ũ	С	J	J
×21	705.7	691.9	716	531.L	172.1,	51.2
×31	711.3	700.3	711	128.6	759.6	423
xL1	2.79	2.80	2.75	3.0	3.0	3.00
×12	0	0	ა	U U	0	O
x22	100	0.60	70	08F	400	230
<b>x</b> <sub>32</sub>	0	0	0	o	0	C
xL2	0.75	0.70	0.70	0.79	0.70	0.70
$f_1(x)$		9.8			0	
f <sub>2</sub> (x)		0			0	
<b>ь(х)</b> (БП	arg)172.12	160.88	170.14	120.69	115.15	145.18

Table 3. Solution Vectors, Puns 3 and L

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		Run 5			Run 6		
	A Raw Vector	B Adjusted Vector	<u>C</u> Graphic Solution	<u>Å</u> Raw Vector	B Adjusted Vector	<u>C</u> Graphic Solution	
Final t	80			90			
× <sub>11</sub>	240	233.0	755	80	78.6	156	
× <sub>21</sub>	10	38.3	Ó	0	υ	0	
×31	1,068.6	1,037.5	1,090	1,158.6	1,139.2	1,134	
×41	1.05	1.15	1.05	1.02	1.05	1 <b>.1</b> 0	
<b>x</b> <sub>12</sub>	0	0	0	0	0	0	
x <sub>22</sub>	591.4	574.4	673	611.4	601.2	638.3	
x.32	60	58.2	0	180	177.0	21.7	
×45	0.55	0.58	0.70	0.16	0.50	0.66	
$f_1(x)$		0			0		
f <sub>2</sub> (x)		58.3			L.O		
l (cb) (x)a	lars)22101	223.45	223.67	225.92	222.15	221.94	

Table 4. Solution Vectors, Runs 5 and 6

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During runs 1 and 2, the graphical solutions were determined in advance. For 3 - 6, however, they were obtained <u>after</u> the adjusted solution had been calculated. (For runs 3 and h, the initial guess turned out to be the solution to the problem.) Tables 3 and h reveal that the algorithm continued to perform in a satisfactory way during the last four runs. For run 6, in fact, the adjusted solution at step 30 indicates a higher net realization than the graphical technique -- $2222.1^{c}$ , as against 2221.9h.

#### 6. Interpretation of results

The numerical parameters used in run 1 for  $p_1$ ,  $p_3$ , and  $q_1$  were considered to be the basic set, and in each subsequent run not more than one of these was altered. In #3 and #4, the value of  $q_1$  was changed; in run 5,  $p_1$ ; and in run 6,  $p_3$ . The adjusted results for all the six runs are summarized by Table 5 in terms of four indicators -- the output of premium grade gasoline, the output of regular grade, the input of TEL, and the refinery realization. These data are also presented on Charts 13-16.

Run 2 differed from #lin only one significant respect. During it, the refiner was not permitted to make stock 3 -- the fictitious intermediate product. The initial blending materials had to be assigned directly to the finished products. In other words, the refiner was not permitted to take full advantage of the concave octane number blending relationship.

This additional restriction had no effect upon the general strategy of converting virtually the entire volume of blending materials into premium grade gasoline. The restriction <u>does</u> have the effect of increasing the TEL requirements, and of decreasing the refiner's not realization.

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The difference in realization at first glance appears small --  $$22^{\circ}.6^{\circ}$ , as against \$230.55 in run 1. However, for a refinery turning out 20,000 barrels of gasoline per calendar day, such a discrepancy would come to an annual figure of roughly \$300,0001. To put the matter another way, the first blending schedule does the same job as the second, with a total TEL requirement that is about 20% smaller. From this, I would conclude that it is eminently worthwhile for a refiner to incur considerable expense in testing gasoline blends, and in attempting to predict the occurrence of curvilinear octane relationships.

In the first run, it turned out that the most profitable blending schedule was one that assigned all 2,000 gallons into premium grade gasoline. This result was quite in line with a rule-of-thumb that is commonly heard among refiners -- to wit, that the maximum profits will be obtained by making the maximum amount of the high-priced product. This rule-of-thumb is not shaken by the results of run 3 or 4. At a q1 availability level of 500 gallons, the best strategy is to produce virtually nothing but premium grade gasoline. At a q1 level of 300 gallons, however, the 3.0 ml. limit on TEL concentration has come into effect. At this low q1 level, the best the refiner can do is to add 3.0 ml. to each gallon of premium grade gasoline, and and to assign the left-over stock 2 to the production of the regular grade product.

The preceding results do not speak well for an alternatively-heard dictum -that the best principal course to follow is to assign 3.0 ml. of ethyl fluid

 $<sup>\</sup>frac{1}{1}$  I do not allege that refiners generally follow such a rule -- only that they say they do.

r(x) (dollars)	Injut of TEL (liters)	Cutput of regular sasoline (gallens)	Output of premium (gallons)	ت <del>ر</del> تر	P1	12,	Run Number	
230°è§	3.752	77.9	1,922.0	•	12	1,000	-	
228-62	4.600	0 <b>.</b> 0	0.020	.23	12	1,000	<b>N</b> 3	
169.88	3.975	0-86	1,202.0		12	500	ىم.י	
115.15	2.950	100.0	ຈມູງ.ບ		21	ۍ د ن	£-	
223.15	1.913	690.7	1,30,3	•23	11.6	1,000	5	
	1.671	782.2	1,217.1	•	12	1,000	0	

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Table 5. Summary of Runs 1 - 6, Adjusted Data

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Fig. 14

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Fig. 16

to each callon of product. Only in making premium grade gasoline during run 3 did it pay to use the maximum allowable TEL concentration.

Runs 5 and 6 cast doubt, not only on the 3.0 ml. principle, but also on the maximum-production-of-premium theory. In run 5, the only parameter change from #1 was a reduction in the price of premium grade product from 12%/gallon to 11.6%. This difference in the price structure is sufficient to bring about a substantial increase in the optimal output of regular grade product -- from less than 100 gallons in #1, to almost 700 gallons in #5. This shift is also accompanied by a marked reduction in the total input of ethyl fluid.

For run 6, a different sort of change in the price structure was tried. The price of ethyl fluid was virtually trebled -- from 0.232/ml. to 0.602. Again comparing the recults with #1, there is a shift into the production of regular grade papoline, and a reduction in the input of study fluid.

To put the matter another way, the rules-of-thumb imply that the same input and output relationships are optimal under all price structures. One of these rules does happen to give a good performance for a particular current set of prices, but does not apply outside thic limited range. Unfortunately, there is no gapy escape. The only way to verify one of these rules-of-thumb in a concrete case is to carry through a detailed formal analysis.

#### 7. Conclusions

At this point, it is appropriate to sum up the findings. On the negative site, the study has demonstrated that certain rules-of-thumb work baily -- even though these principles have occasionally been put iorward by men in the refining industry. The study, moreover, has shown P=383 =32=

that the optimal input and output relationships will be intimately linked with the price structure. Figures 13 and 14 give some clues as to the nature of this linkage. Before the economist jumps to the conclusion that these really are supply and demand curves, however, he is urged to reread the caveats of Section 3.

On the positive side, the claims are necessarily more cautious. The study indicates that a refiner will do well to make a careful investigation of his gasoline stocks for non-linear blending characteristics. The results do not imply that a 20% saving in TEL costs will inevitably occur.

More significant from a long-range viewpoint, the computing runs indicate that it is possible to solve concave programming problems on a digital computer. The particular procedure employed is undoubtedly wasteful of machine time, and superior methods will surely evolve. The next programming problem that will be attacked is one that has been formulated by one of the major west Coast refiners. Although this coming problem has  $22 x_i$  and  $8 u_j$ , the basic notion is the same. The quantities available of various blending stocks will be taken for granted, and the analysis carried on from that point. Certain cutting temperatures will also enter as independent variables. At a later date, it is expected that the model will be expanded to incorporate such process variables as reactor temperatures and recycle ratios.

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### Appendix I. Constants for Six Sets of Calculations

			Sources:
Р1 N1		12¢/ <u>ral.</u> ) ) ) 70 octane )	Ref. 8 gives the following Gulf Coast, bulk cargoes price range for 90 octane (ASTM Research) promium motor gasoline: 11.75 - 12 - 12.25¢/gal. These prices
·		numbe <b>r</b> ))	were in effect on November 21, 1952.
P2	£	11¢/gal. ) ) )	Ref. 8 gives the following Gulf Coast, bulk cargoes price range for 53 octane (ASTM Research) regular motor gasoline:
N2		83 outane ) number ) )	10.75 = 11 = 11.25%/gal. These prices were in effect on November 21, 1952.
P3	=	0.23¢/ml. of ) TEL ) )	The Los Angeles Sales Office of the Ethyl Corporation gave this quotation on Nevember 21, 1952. It applies to motor mix ethyl fluid, delivered in tank-car lots to any U. S. destinution.
41	=	300, 500, 1,000 gal. ) of catalytic-cracked-) plus-polymer pasoline)	Ref. 9, p. 5 indicates the following smake down of U. S. bracking plant capacity as of January 1, 1952:
¢5	Ξ	1,000 gal. of thermal) crocked paraline ) )	thermal cracked: /?L,69t ) arrels/day; catalyt cracked (asoline: 907,544 tarrels/ day.
			N.B. There are wide variations in the ratio of thermal to catalytic capacity as between individual refinences and

refining regions.

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Appendix I. (continued)

The  $a_i$ ,  $b_i$ , and  $c_i$  coefficients for each stock were derived from the bogen and Nichols data [1, Table II, p. 2630]. The three sets of observations are shown on Figure 1. The individual coefficients had the following numerical values:

Stock #	1	2	٤
ai	٥٢•٦	89.6	94.1
b <sub>i</sub>	.233	<b>.</b> L33	•266
C,	-8.931	-12.13	-9.0K

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lun fumber	1	2	3	L	5	6
× <sub>11</sub> (٥)	0	1,000.0	U	0	()	U
$\mathbf{x}_{\hat{\mathbf{c}}1}(v)$	Э	1,000.0	7.5 <b>.7</b>	471.4	<u>0</u>	J
x -1(0)	U	υ	714.3	1.28.6	1,128.6	1,129.6
x <sub>l,1</sub> (0)	U	<b>5</b> •20	2.0	3.0 -	1.2	1.2
x <sub>lč</sub> (J)	Q	0	υ	U	- O	0
x <sub>22</sub> (0)	0	0	Û	100.0	571.L	571 <b>.</b> 4
×32 <sup>(0)</sup>	0	0	0	0	0	0
x <sub>12</sub> (0)	О	Ο	0	0 <b>.7</b>	0.7	0.7
u <sub>l</sub> (0)	10.00	12.20	12.10	12.00	12.10	12.1.
u <sub>2</sub> (0)	10.00	10.75	10.75	11.00	10.75	10.75
u3(0)	0 <b>.1</b> 00	0.151	0.154	0.216	0.154	0.154
u <sub>L</sub> (C)	0 <b>.1</b> 60	0.03	0.154	0.052	0.154	0.154

Appendix II. Initial Vectors for Six Sets of Calculations

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Addendum to P-383, "Concave Programming for Casoline Blends"

In discussing P-383. Dr. Martin beckman uncovered a problem to which I had not previously given attention. He has made the point that for a function of many variables, f(x), to be truly concave, it is necessary but not sufficient for that function to be concave in each variable taken separately.

The basic problem arises out of the fact that the function xy is neither concave nor convex - for nonnegative independent variables x and y. This is despite the fact that it is concave and convex in either variable separately.

**Proof:** Consider two points  $(x_1, y_1)$  and  $(x_2, y_2)$ . Convexity would require:

(1) 
$$\left[\begin{array}{c} \mathbf{x}_{1} + \mathbf{x}_{2} \\ -\frac{\mathbf{x}_{2}}{2} \end{array}\right] \left[\begin{array}{c} \mathbf{y}_{1} + \mathbf{y}_{2} \\ -\frac{\mathbf{y}_{2}}{2} \end{array}\right] \leq \frac{1}{2} \mathbf{x}_{1} \mathbf{y}_{1} + \frac{1}{2} \mathbf{x}_{2} \mathbf{y}_{2}$$
  
 $\left[\begin{array}{c} \mathbf{x}_{1} + \mathbf{x}_{2} \\ -\mathbf{x}_{1} + \mathbf{x}_{2} \end{array}\right] \left[\begin{array}{c} \mathbf{y}_{1} + \mathbf{y}_{2} \\ -\mathbf{y}_{1} + \mathbf{y}_{2} \end{array}\right] \leq 2\mathbf{x}_{1} \mathbf{y}_{1} + 2\mathbf{x}_{2} \mathbf{y}_{2}$   
 $\mathbf{x}_{1} \mathbf{y}_{2} + \mathbf{x}_{2} \mathbf{y}_{1} \leq -\mathbf{x}_{1} \mathbf{y}_{1} + \mathbf{x}_{2} \mathbf{y}_{2}$ 

(2)  $\mathbf{x}_1 (\mathbf{y}_2 - \mathbf{y}_1) \leq \mathbf{x}_2 (\mathbf{y}_2 - \mathbf{y}_1)$ 

For nonnegative x and y, and for  $y_2 > y_1$ , expression (2) requires  $x_1 \le x_2$ . But the convexity condition applies to any arbitrary  $(x_1, y_1)$  and  $(x_2, y_2)$ . This is a contradiction. Similarly for concavity. Q.E.D.

Now, what are the implications of this result for the gasoline blending model? Fortunately, it turns out that by a re-definition of variables, the payoff function g(x) can be made concave -- indeed linear. Unfortunately, though, this re-definition does not lead to any rigorous proof of the concavity of restraint

equations (9) and (10). On the contrary, it shows up the possibility of non-concavity in these restraint conditions when two of the blending stocks have widely divergent lead susceptibilities.

Let us define new variables,  $x_{j1}$  and  $x_{52}$ , in the following way:

$$\mathbf{x}_{51} = \mathbf{x}_{41}(\mathbf{x}_{11} + \mathbf{x}_{21} + \mathbf{x}_{31})$$
$$\mathbf{x}_{52} = \mathbf{x}_{12}(\mathbf{x}_{12} + \mathbf{x}_{22} + \mathbf{x}_{32})$$

Equation (3) can now be transformed into a linear form involving the two new variables,  $x_{51}$  and  $x_{52}$ :

$$(3a) g(x) = p_1 (x_{11} + x_{21} + x_{31}) + p_2 (x_{12} + x_{22} + x_{32}) - p_3 (x_{51} + x_{52})$$

To simplify the discussion of equations (9) and (10), I shall arbitrarily assume that both  $x_{31}$  and  $x_{32}$  are constrained to be zero, and will focus attention on the function  $f_3(x)$ , dealing with the octane specification of the premium grade gasoline. Suppose that the octane numbers and the quantities available of the two blending stocks had been as follows:

	Stock 1	Stock 2
Quantity available, x <sub>11</sub>	1,000 gal.	1,000 gal.
Octane number, clear	···!+ . O	90.09
Octane number, with 3 ml. of TEL	0.0	94.8
Number of ml./gal. required for $90$ octane leaded gasoline, $x_{i_{1}}$	3.0	• 0
Total number of ml. required for $20$ octane leaded gasoline, $x_{c1}$	3,000	0

Assuming straight line interpolation at constant lead levels for the two stocks, and assuming a 50-50 blend, we come up with these results for the blend:

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Quantity available, $(x_{11} + x_{21})$	2,000 gal
Octane number, clear	82.0
Octane number, with 3 ml. of TEL	92.4
Number of ml./gal. required for $90$ octane leaded gasoline, $x_{41}$	1.6
Total number of ml. required for 90 octane leaded gasoline, x <sub>51</sub>	3,200

In other words, if the two initial materials are ethylized and marketed separately, the average TEL requirement per gallon comes to 1.5 ml. If the two are blended together, the same amount of premium gasoline is produced, but the average lead requirement increases to 1.6 ml. This behavior clearly violates conceivity of the function  $f_3(x_{11}, x_{21}, x_{31}, x_{51})$ , and leads to the possibility of multiple isolated maxima. Lacking the concavity property in our functions, we may be led to adopt blending achedules that are locally optimal, but which do not, in fact. represent the best of all solutions available.

Now, how zerious are the possibilities of such local maximm? The problem cannot be shrugged off, but I believe that in most particular applications these local extrems can be detected by the investigator. In order for the violation of concavity to take place, some of the blending material must be particularly high in lead susceptibility, and some of it must be extremely low. In addition, the first material must require a high TEL concentration in order to meet the specification, and the second a low TEL level Enowing something about the occurrence of such pitfalls, the intelligent refiner should be able to avoid ensnarement.

The difficulties arising out of non-concavity are not unique to the programming method described in P-383. The same argument would apply if

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 $x_{l_{1}}$  and  $x_{l_{12}}$  were taken as parameters, and a separate linear programming problem then run off for each of many <u>combinations</u> of the two. This difficulty would arise in the case of any trial-and-error method that consisted in changing one variable at a time, and observing the effects upon the payoff, g(x). And finally, such failure of the proper curvature conditions could frustrate an optimization via a Lange-Lerner shadow price market mechanism.

The dilemma raised by Dr. Beckman should not be viewed as an absolute impasse, but rather as a challenge to the ingenuity of workers in this field. These latter can take comfort in recalling that truly rigorous analysis is seldom applicable within the domain of applied mathematics.



Mr. Lloyd Philipson has pointed out the following misprints:

last line of p. 12 should read: "If  $u_j(t) + \Delta u_j \ge 0$ , then  $\Delta u_j = \Delta u_j(t)$ "

line 6 of p. 13 should read: "If  $\frac{\partial \phi(t)}{\partial x_i} < 0$ , then the 'candidate'  $\hat{\Delta x_i} = -k_i$ "

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