IDENTIFICATION AND OPTIMIZATION OF MANAGEMENT AND ENVIRONMENTAL SYSTEMS

by 45

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INTRODUCTION

The main purpose of this thesis was to identify parameters in management models and to apply system technique to simulate and optimize environmental systems. This thesis consisted of two parts with each part devoted to one of the above two fields.

In the identification of parameters, the coefficients in advertising models were estimated. One coefficient was estimated from an advertising model. Then two and three coefficients were estimated from another advertising model which was a more practical model of the former. These coefficients were estimated from the generated data of the models. There was one set of generated data for one coefficient estimation and another set of generated data for two and three coefficients estimation. In each case the original generated sets of data were first used; then random noise was imposed on the generated data. Two methods, Quasilinearization, and numerical integration and search were used to identify these parameters.

In the simulation and optimization of environmental conditions, the work was based mainly on Fanger's comfort equation. The comfort equation was carefully studied. Simulation was done to obtain the feasible region of the comfort equation. The system was then optimized using the comfort equation as one of the constraints. In addition, velocity and relative humidity constraints were used. Simplex search technique was used for the optimization calculations.

PART I: PARAMETER IDENTIFICATION

INTRODUCTION

In all branches of contemporary science the challenges were description and prediction. Observing certain phenomena it was desired to describe what had happened and the subsequent behaviour. Upon examining a physical system and performing various kinds of qualitative and quantitative experiments, a series of data were obtained from which arose a set of desired state variables which could be represented by a vector $h(x)$. To describe the system and its output it would be required to choose a model or a function constituting the vector $h(x)$, which must yield a solution that fits the observed facts, qualitatively or quantitatively, to within an experimental error or within an accuracy sufficient for the purpose. This was the inverse problem - given a set of data, it was required to find the equations that yielded these values.

The differential equations served as a connection between a simple physical law and a frequently complex relation of several variables. In those processes where continuous changes in the values of the variables occurred a differential equation represented the correct relation between the local values of the variables and their rate of change. The relation between the dependent and independent variables was continuous.

The origin and development of differential equations had always been closely associated with applications. The law of nature in many fields of science were formulated in terms of differential equations. The same type of differential equation often described unrelated physical phenomena. Thus, differential equation served as a unifying thread connecting the .

various parts of science. In this connection, the application of differential equations were found in every field of science and engineering. To name a few they were used to describe chemical reactions, electrical circuit, mechanical vibrations and planetary motions. In Industrial Engineering they were used to describe the effect of advertising on sales and profits; the inventory, production and replacement problems.

However, in engineering applications, after a function, or a model had been set up in the form of differential equations it was often necessary to estimate the parameters or coefficients. Generally the parameters could not be measured directly. The only measurable variables were usually the dependent variables of the differential equations. Unfortunately, in most cases the differential equations could not be solved analytically. Thus, it was desirable to determine the parameters from the output of a system.

The identification of parameters in dynamic systems represented by differential equations had been under extensive investigation in fields such as Chemical Engineering and Control Engineering, but to the knowledge of the author little work had been done in Industrial Engineering. The purpose of this work was to use the recently developed techniques to identify parameters in a management model in Industrial Engineering.

The parameter estimation was treated as a multi-point boundary-value problem in this work. Two methods, quasilinearization, and numerical integration and search were used to identify the parameters.

The computation times shown at the end of each of the table were approximations only. It could be seen that in some cases less time was registered even though more evaluation were made in the search. This was due to the fact that less printouts were made.

STATEMENT OF PROBLEM

Parameter identification was a combination of experimental work with mathematical analysis. A model consisting of systems of equations was formed to describe a system. Experiments were carried out to obtain a series of data. From the data the coefficients of the equations were obtained by mathematical techniques. This work concerned mainly with the mathematical aspects and is restricted to models which can be represented by ordinary differential equations. The data were generated mathematically.

There were three types of problems in parameter estimation: the estimation of constant parameters, time varying parameters, and finally the general concept of differential approximation.

Based on the initial knowledge of the process, the identification problem could be interpreted in two ways [17].

Identification: The process was considered as a "black box" where only the inputs and outputs were known.

Parameter estimation: The performance equations of a system were known but the parameters of those equations were unknown.

The first interpretation gave a very general viewpoint and many theories could be developed to give the stimpulated inputs and outputs to a certain desired accuracy. The second was more realistic and more practical. For illustrative purposes, an advertising model was considered [23],

$$\frac{dK(t)}{dt} = cK(t)\left|1 - \frac{K(t)}{N}\right|$$

where

$K(t)$ = number of informed participants at time t.

$K(0)$ = number of informed participants in the group at time 0.

c = contact coefficient; the number of contacts made by one informed person per unit time, and

N = total number of participants in the group at time t.

In the above advertising model, c was an unknown quantity and was to be determined experimentally by measuring the informed participants, K, at various times t. In other words, by using the following measured or experimental values

$$K^{(exp)}(t_s) = b_s \qquad S = 1, 2, \ldots, m_1,$$

with $m_1 \geq 1$ and $0 \leq t_s \leq t_f$, it was desired to determine the unknown parameter c. The quantities b_s were known values and were obtained by measuring K experimentally at various times t_s. The number of the experimental values, m_1, must be greater than or equal to the number of unknown constant parameters. The superscript (exp) indicated K to be experimental values.

LITERATURE SURVEY

The techniques employed to identify constant parameters from experimental data could be summarized by the following six methods [10]:

1. Analytic (exact or approximate) integration of the set of differential equations, and subsequent application of iterative nonlinear least-squares regression techniques.

Kittrell et. al. [14] reviewed a method which allowed data points to be chosen in such a fashion that precise estimates of the parameters in nonlinear reaction rate models could be obtained. This method allowed each future data point to be selected such that the confidence region of the

estimated parameters was smaller with it than with any other possible data point within the region of experimentation. This procedure was applied to Hongen-Watson models with hypothetical experimental data. It was found that for the same number of data points, the parameters in the model could be estimated eighteen times more precisely by using this suggested experimental data than by another commonly used design. It was found that the positions of the data points in the well-designed experiments were more sensitive to the functional form of the model than to the current estimates of the magnitudes of the parameter values.

The specific model used was:

$$\gamma = \frac{K\, K_A\, K_B\, p_A\, p_B}{(1+K_A\, p_A + K_B\, p_b)^2}$$

The hypothetical data points utilized in this example were constructed by using $K = 4.94 \times 10^{-4}$ g-mole/(g - catalyst) (min), $K_A = 14.64$ atm^{-1} and $K_B = 19.00$ atm^{-1} as the time parameter value in the above equation.

2a. Differentiation of the empirical data directly and subsequent application of linear least-squares regression technique:

The design of kinetic experiments had been considered as a problem in selecting the best time intervals for measuring the composition of the reacting mixture in Chemical Engineering. Lindsay [18] made a study on the best time intervals so that the rate constants in a chemical reaction could be best estimated. He transformed the time variable to a dimensionless variable, θ. This transformation led to a time schedule for making composition measurements which resulted in a reasonably close approach to equal changes in composition with successive integral changes in θ throughout the

entire time range of the experiment. This minimized the number of measurements required for evaluating a rate constant to a desired level of accuracy and permitted facile calculation of the instantaneous reaction rate by methods of numerical differentiation. This method could be applied to almost any reaction regardless of whether or not the form of the rate equation was known in advance.

2b. Linear regression to fit the empirical data, differentiation of empirical regression equation, followed by linear regression to estimate the coefficients.

3a. Numerical integration of the set of differential equations using empirical data directly, followed by iterative nonlinear least-squares:

Ball and Groenweghe [1] made a study on the determination of best-fit rate constants in chemical kinetics. The following example of second-order kinetics were considered:

$$C_0 + C_2 \overset{k_1}{\underset{\leftarrow}{\rightarrow}} C_1 + C_1$$

$$C_1 + C_3 \overset{k_2}{\underset{\leftarrow}{\rightarrow}} C_2 + C_2$$

$$C_2 + C_4 \overset{k_3}{\underset{\leftarrow}{\rightarrow}} C_3 + C_3$$

$$C_0 + C_3 \overset{k_4}{\underset{\leftarrow}{\rightarrow}} C_1 + C_2$$

$$C_1 + C_4 \overset{k_5}{\underset{\leftarrow}{\rightarrow}} C_2 + C_3$$

$$C_0 + C_4 \overset{k_6}{\underset{\leftarrow}{\rightarrow}} C_1 + C_3$$

The problem was to find $k_1, \ldots, k_6$ such that $S = \sum_{n=0}^{N} \sum_{j=1}^{M} (c_{ij} - C_{ij})^2$ has a minimum value where C_{ij} indicated measured concentration of component C_i at time t_j. Initial concentrations, c_{i0}, assumed to be exact (based on weighting of reactouts) and C_{ij} indicated concentration of component i at time t_j computed from kinetic model. The problem separated into two major parts: the computation of the c_{ij} values and the methods used to minimize S. The first was solved by numerically integrating the appropriate differential equations with Fehlberg's predictor-corrector type [8]. The second part of the problem was solved by a method proposed by Marquardt [19] who combined the best features of the Gauss-Newton and the steepest descent methods. The Gauss-Newton method was characterized by rapid (second order) convergence when sufficiently close to the final solution points. The steepest descent method functioned no matter how far away the starting point was from the solution. However, it converged very slowly when the solution was near. Thus, the proper combination of these two methods would allow fast convergence regardless of the starting point.

Cull and Brenner [6] applied nonlinear regression to kinetics of Hexane Isomerization. First, the differential equations were solved numerically using the assumed values of the rate constants to obtain calculated values of isomer concentrations to compare with the experimental data. An initial "sum of the squares" was then obtained by squaring the deviations between the calculated and experimental values and summing them. The object of this regression was to obtain the rate constants that minimized the sum of squares.

The next step was to find the rate constant that would decrease the sum of squares. This was done by changing each rate constant by a small amount

and evaluating the effects of these changes on the sum of squares. This was carried out through a process of numerical differentiation in which the equations were expanded in a Taylor's series, retaining only the linear terms. This produced a new system of equations (one for each data point) which were linear and were described as "correction factors." Linear regression method was then used to determine statistically the best values of these correction factors. From these correction factors, new values of rate constants were calculated, which would be used as the new initial values. The entire process was repeated until the best values of rate constant that minimized the sum of squares was obtained.

Himmelblau et. al. [10] made a study on the determination of kinetic rate coefficients for complex reactions by user-oriented iterative methods. The differential equations representing the reaction system was nonlinear in the dependent variable but the coefficients were linear. Direct integration of the model for a sequence of time steps permitted the model coefficients to be estimated by minimizing the sum of the squares of the weighted deviations. Three weighting schemes were compared. The model used could be abbreviated as:

$$\frac{dC_j}{dt} = \sum_{k=1}^{N} B_k R_{j,k} \quad (j = 1, 2, \ldots, M)$$

C = dependent variables

B = kinetic coefficients presumed constant

R = represented any desired function of C and t

If each of the above equation was integrated with respect to time from t_0 to t_i, the following equation arose

$$C_j(t_i) - c_j(t_0) = \sum_{k=1}^{N} B_k \int_{t_0}^{t_i} R_{j,k}\, dt \qquad \begin{matrix} i = 1, 2, \ldots, P \\ j = 1, 2, \ldots, M \end{matrix}$$

where

P = number of time intervals between the times at which the concentrations were measured.

which could be abbreviated as

$$Y_{ig} = C_{ig} - c_{0g} = \sum_{k=1}^{N} B_k X_{ijk}$$

where B_k were linear coefficients to be determined.

The criteria used to estimate the B_k's was to minimize the sum of the squares of the weighted deviations.

$$DN_{ij} = (Y_{ij} - \hat{Y}_{ij})\, W_{ij}$$

Y_{ij} = measured experimental values of the dependent variables.

$\hat{Y}_{ij}$ = predicted values of the dependent variables.

W_{ij} = weighting factor associated with each deviation

Weights used were:

A. $W_{ij} = 1$. Equal weight was given to each D_{ij}

B. $W_{ij} = \dfrac{1}{|Y_{ig}|}$ Each absolute deviation was converted into a relative deviation.

C. $$W_{ij} = \left| \sum_{L=1}^{P} \left(Y_{Lj} - \left(\frac{1}{P}\right) \sum_{i=1}^{P} Y_{ij}\right)^2 \right|^{-\frac{1}{2}}$$

Each weight was related to the variance of Y_{ij}.

Simulation studies and tests with actual data indicated that the proposed technique was effective.

3b. Linear regression to fit the empirical data, followed by numerical integration of the set of differential equations.

4. Trial and error search using analog computers to match the empirical data. [13]

5. Method of differential corrections.

Howland and Naillancourt [11] studies a generalized curve-fitting procedure by the differential corrections method. The procedures were reproduced below:

It was supposed that the system

$$\ddot{Y} = \phi(y, \dot{y}, t, \alpha_k) \quad 1 \leq k \leq m \tag{1}$$

of n ordinary differential equations, together with the initial conditions $y(\tau) = \beta$, $\dot{y}(\tau) = \gamma$ define the column-vector $y(t, \alpha, \beta, \gamma)$ of functions which depend upon the parameters α_k, β_j, γ_j $(1 \leq k \leq m, \quad 1 \leq j \leq n)$. It was supposed also that values of some solution of (1), corresponding to unknown values of the parameters, were tabulated at given points t_1, t_2, t_3, ..., t_p, where $p > 2n + m$. From these given data the differential corrections were used to determine the parameters.

This method could be used to determine chemical constants as well as force constants in aerodynamic derivatives in mechanical problems.

6. Quasilinearization

Lee [16] formulated the estimation problem as a two-point or multi-point boundary-value problem. The classical least squares was used. To illustrate the approach, the Peclet group and the reaction rate group in a tubular reactor with axial mixing were obtained. Parameters P and R were identified in the following system of equations by Quasilinearization

$$\frac{dx}{dt} = y$$

$$\frac{dy}{dt} = Py + PR\lambda^2$$

The exact parameters were P = 6 and R = 2. Two sets of initial approximations of parameters were used: 1,1 and 5,5. Ten numerical values were used as experimental data. Both sets converged at the eighth iteration.

Bellman et. al. [2] used the Quasilinearization and the sum of squares of the deviations to identify α_i and ω_i in the following system.

$$f(t) = \sum_{i=1}^{R} \alpha_i \operatorname{Cos} \omega_i t$$

In the approach it was considered that the N-dimensional vector X(t) was a solution of the differential equation $\dot{X} = f(X, a)$, $X(0) = c$, where the system parameter vector a and the initial state vector c were unspecified. At certain times the system was "observed" which resulted in the approximate conditions $(\beta_i, X(t_i)) \cong b_i$, $i = 1, 2, \ldots, M \geq N$. It was desired to determine the vectors a and c so that the sum of the squares of the deviations

$$S = \sum_{i=1}^{M} \{(\beta_i, X(t_i)) - b_i\}^2$$

was minimized. In another word, the problem was to determine the initial conditions c and $a^{(0)}$ so as to minimize S. This problem was solved by the quasilinearization approach.

Bellman et. al. [3] also applied Quasilinearization to the estimation of chemical rate constants using raw kinetic data, obtained by Bodenstein and Lindner [5], on some gas phase reactions of nitrogen and oxygen.

The descriptive differential equation after various normalizations had the form

$$\frac{dx}{dt} = k\,(a-x)(b-x)^2 - kx^2$$

$$a = 126.2$$

$$b = 91.9$$

where k and κ were the rate constants to be estimated on the basis of the experimental data.

The solution converged after the fourth iteration using less than 30 seconds on an IBM 7044. The initial and final estimates of the parameters were $k_0 = 1 \times 10^{-6}$; $\kappa_0 = 1 \times 10^{-4}$ and $k_4 = .4577 \times 10^{-5}$ and $\kappa_4 = .2797 \times 10^{-3}$ with $.210 \times 10^{-2}$ as the sum of the squares used. Bodenstein and Lindner [5], using a combination of chemical theory and the experimental observation estimated that $k = .53 \times 10^{-5}$ and $\kappa = .41 \times 10^{-3}$ with $.555 \times 10^{-2}$ as the sum of the squares of deviations.

Bellman et. a. [4] applied Quasilinearization to system identification and prediction. In the illustration the Van Der Pol's equation [22, 9] shown below was solved

$$\dot{X} = \mu$$

$$\dot{U} = -\lambda(X^2 - 1)\,\mu - X \qquad (1)$$

where X was a scalar and λ was an unknown constant. Three experimental data were obtained.

$$X(4) = -1.80843$$
$$X(6) = -1.63385 \qquad (2)$$
$$X(8) = -1.40456$$

It was desired to determine the unknown values of λ and both x and μ for i = 4.

The system of equations became

$$\dot{X} = \mu$$

$$\dot{\mu} = -\lambda(X^2 - 1)\,\mu - x \qquad (3)$$

$$\dot{\lambda} = 0$$

and two sets of initial approximations were used:

$$X(4) = -1.80843$$
$$\mu(4) = 0.08$$
$$\lambda(4) = 7.0$$

and

$$X(4) = -1.80843$$
$$\mu(4) = 0.1000$$
$$\lambda(4) = 5.0000$$

With first set of initial approximations the solution converged at the end of the fourth iteration, while the second set converged at the end of the sixth iteration.

A trial was made with the initial estimate of the system parameter 20. It resulted in an overflow.

Donnelly and Quon [7] made a study on the computation of "best fit" parameters in non-linear mechanistic rate equations using Quasilinearization and data perturbation. The complete set of differential equations under study was

$$\frac{d\underline{x}_j}{dt} = \underline{f}_j(\underline{X}_j, \underline{a}, t) \quad j = 1, \ldots, n$$

$$\frac{d\underline{a}}{dt} = \underline{0} \quad \underline{0} \text{ was of order } q \times 1$$

Initial conditions

$\underline{X}_j(0)$ unspecified for $j = 1, \ldots, n$

$\underline{a}(0)$ unknown

$\underline{x}_j$ = state vector for jth experiment

$\underline{a}$ = vector of system parameters

The procedure was to guess an initial trial vector $\underline{a}(0)$. With this the above equation was integrated to obtain $X_{ijk}^{(0)}$, the value of the i^{th} state variable at t_{jk}, for all points at which observed data $\hat{X}_{ijk}$, the measured value of the i^{th} state variable at t_{jk}, were available. If the initial trial vector $\underline{a}(0)$ resulted in a set of $X_{ijk}^{(0)}$ "close enough" to X_{ijk}, then

Quasilinearization technique would converge. If not then the original problem was modified by perturbing the data as follows:

$$\hat{X}^{(1)}_{ijk} = \hat{X}^{(0)}_{ijk} + \alpha(\hat{X}_{ijk} - X^{(0)}_{ijk}$$

$$0 \leq \alpha \leq 1.0$$

The perturbed data thus fall between the observed and predicted data. The choice of $\alpha = 1.0$ gave rise to the original algorithm.

Method 1 might work successfully for small sets of simple equations but was not practical for realistic models. Method 2 used linear regression analysis, but the differentiation of empirical data increased the existing inherent errors in the experimental data and in practice Method 2 was not satisfactory. Method 4 was tedious and did not lead to clear cut measures of "best fit".

Two methods were proposed in this work--Quasilinearization and numerical integration and pattern search. These two methods fell in the third method. The former was similar to Bellman [3] and Lee [17].

ONE PARAMETER IDENTIFICATION

A constant parameter in a simple advertising model was identified here. Two methods, quasilinearization and numerical integration and pattern search were used to identify the parameter. The experimental data was generated by actually solving the model numerically. Later, the effect of noise in the data was studied with the same technique.

A. The Model

The model for one parameter estimation was formulated below [23]:

Consider a group of people only certain member possessed a particular piece of information. The total number of persons in the group under consideration remained constant and that diffusion of information occurred through advertising. The number of "contacts" made by an advertisement in an arbitrary unit of time was given by a contact coefficient; this coefficient was a fixed number which was assumed to be the same for all members of the group. In a contact, the contacter received the information if he did not have it yet. If he already had it, the contact was wasted so far as increasing the number of people who had the information was concerned.

Let $K(0) \equiv K_0$ = number of informed participants in the group at time 0.

N = total number of participants in the group.

c = contact coefficient; the number of contact made by one informed person per unit time, and

K(t) = number of informed participants at time t.

Then

$\frac{K(t)}{N}$ = proportion of informed persons in the group at time t.

$1 - \frac{K(t)}{N}$ = proportion of "uninformed" persons in the group at time t.

$cK(t)dt$ = contacts made during a time interval dt.

The increase in the total number of informed during a short interval of time dt was obtained by multiplying the number of contacts by the persons who did not posses the information, since only contact with uninformed group members led to an increase in informed members [23].

$$dK(t) = cK(t)dt\ (1 - \frac{K(t)}{N})$$

which resulted in the differential equation:

$$\frac{dK(t)}{dt} = cK(t)\left|1 - \frac{K(t)}{N}\right| \qquad (1)$$

The parameter to be identified from generated data without and with noise was the contact coefficient c which was defined as the number of contacts made by one informed person per unit time.

For a particular article and means of communication the above model described the rate of change of informed persons at any time t. In the model the number persons, N, and the number of informed persons, K(t), at any time t could be obtained by research or by conducting a survey. K(t) would be the measured data and from which parameter c could be estimated. It was desirable to estimate c because it reflected the effectiveness of the means of communication. In another way, by controlling c a desired K(t) could be obtained. In this way parameter c would dictate the means of communication to be used for a desired number of informed persons.

B. Deterministic Model Without Noise

B-1. Experimental data generation

The experimental data was generated by actually solving equation (1) with Rurge-Kutta-Gill numerical integration.

The following constants and step size were used which gave a 1% error by numerical integration.

K(0) = 100 informed persons at time 0.

N = 1000 persons in the group

c = 2 persons / unit time

$t(0)$ = 0 initial time

t_f = 5 final time

Δt = .05 integration step size

$K(T)$ = 999 informed persons at final time T.

The relationship between time t and informed persons $K(t)$ was shown in Table 1.

B-2. Quasilinearization

In this section the contact coefficient, c, in equation (1) was identified by Quasilinearization and the least square criterion. The model was reproduced as below

$$\frac{dK(t)}{dt} = c\ K(t) \left[1 - \frac{K(t)}{N}\right] \tag{2a}$$

It was convenient to consider the unknown parameter c as a dependent variable and as a function of the independent variable t. In addition to equation (2a) the constant unknown parameter could be represented by the following differential equation [4]

$$\frac{dc}{dt} = 0 \tag{2b}$$

The initial condition was $K(0) = 100$ (3)

Since the experimental data was more than one the classical least squares criterion was used. The object was to determine the parameter c so that the sum of the squares of the deviations as shown below was minimized.

Table1. GENERATED DATA WITHOUT NOISE FOR ONE PARAMETER IDENTIFICATION

TIME	INFORMED PERSONS	TIME	INFORMED PERSONS	TIME	INFORMED PERSONS	TIME	INFORMED PERSONS
0.00	100.00	0.05	109.37	0.10	119.49	0.15	130.42
0.20	142.19	0.25	154.83	0.30	168.37	0.35	182.84
0.40	198.26	0.45	214.63	0.50	231.97	0.55	250.26
0.60	269.49	0.65	289.62	0.70	310.62	0.75	332.42
0.80	354.98	0.85	378.19	0.90	401.97	0.95	426.23
1.00	450.85	1.05	475.71	1.10	500.69	1.15	525.66
1.20	550.51	1.25	575.11	1.30	599.35	1.35	623.10
1.40	646.28	1.45	668.79	1.50	690.56	1.55	711.51
1.60	731.59	1.65	750.77	1.70	769.01	1.75	786.29
1.80	802.61	1.85	817.97	1.90	832.39	1.95	845.89
2.00	858.48	2.05	870.20	2.10	881.08	2.15	891.16
2.20	900.49	2.25	909.10	2.30	917.03	2.35	924.33
2.40	931.03	2.45	937.18	2.50	942.82	2.55	947.98
2.60	952.69	2.65	957.00	2.70	960.93	2.75	964.52
2.80	967.79	2.85	970.76	2.90	973.47	2.95	975.93
3.00	978.17	3.05	980.21	3.10	982.06	3.15	983.74
3.20	985.26	3.25	986.64	3.30	987.90	3.35	989.04
3.40	990.07	3.45	991.01	3.50	991.85	3.55	992.62
3.60	993.32	3.65	993.95	3.70	994.52	3.75	995.04
3.80	995.51	3.85	995.94	3.90	996.32	3.95	996.67
4.00	996.99	4.05	997.27	4.10	997.53	4.15	997.76
4.20	997.98	4.25	998.17	4.30	998.34	4.35	998.50
4.40	998.64	4.45	998.77	4.50	998.89	4.55	998.99
4.60	999.09	4.65	999.17	4.70	999.25	4.75	999.32
4.80	999.39	4.85	999.44	4.90	999.50	4.95	999.54
5.00	999.59						

$$Q = \sum_{S=1}^{m_1} \left| x(t_S) - b_S \right|^2 \tag{4}$$

where the minimization was over the parameter c and $x(t_S)$ was obtained by solving equation (2).

The system (2) and (3) formed a multi-point boundary-value problem.

B-2a. Computational Procedure

The parameter estimation problem could now be approached by the quasilinearization technique.

Since the right hand side of equation (2) was nonlinear and the boundary condition was the initial type, the Runge-Kutta-Gill numerical integration could be applied directly. The recurrence relation for the system of equations was obtained from equation (10) in Appendix I, Part I.

$$\frac{dK_{n+1}(t)}{dt} = c_n k_n \left(1 - \frac{K_n}{N}\right) + (K_{n+1} - K_n)\left(c_n - \frac{2c_n K_n}{N}\right) + (c_{n+1} - c_n)\left(K_n - \frac{(K_n)^2}{N}\right) \tag{5a}$$

and

$$\frac{dc_{n+1}(t)}{dt} = 0 \tag{5b}$$

Here the subscript n denoted the nth iteration. In equations (5) K_{n+1} and c_{n+1} were considered as unknown functions of t; K_n and c_n were considered as known functions of t obtained from the (n-1)st iterative solution. The above equations became two simultaneous first order linear differential equations. Since the system of equations (5) was linear, it could be solved

by the use of the principle of superposition [16]. With one initial condition (3) given, only one set of homogeneous solution was needed for the two equations in (5). Thus, the general solution of equation (5) were:

$$K_{n+1}(t) = K_{p,n+1}(t) + A_{1,n+1}\, K_{h1,n+1}(t) \tag{6a}$$

$$c_{n+1}(t) = c_{p,n+1}(t) + A_{1,n+1}\, c_{h1,n+1}(t) \tag{6b}$$

where subscript p indicated particular solutions and h_1 denoted the first set of homogeneous solutions. $A_{1,n+1}$ was an integration constant to be determined from the simplex search technique. Equation (6) could be written in matrix form:

$$K_{n+1}(t) = K_{p(n+1)}(t) + K_{h(n+1)}(t)\, A_{n+1} \tag{7}$$

The state vector $K_{n+1}(t)$ and the particular solution vector $K_{p(n+1)}(t)$ were defined as:

$$K_{n+1}(t) = \begin{vmatrix} K_{n+1}(t) \\ \\ c_{n+1}(t) \end{vmatrix}, \quad K_{p(n+1)}(t) = \begin{vmatrix} K_{p,n+1}(t) \\ \\ c_{p,n+1}(t) \end{vmatrix} \tag{8}$$

The homogeneous solution matrix was defined as

$$K_{h(n+1)}(t) = \begin{vmatrix} K_{h1,n+1}(t) \\ \\ c_{h1,n+1}(t) \end{vmatrix}$$

The particular and homogeneous solutions were chosen in such a way that they satisfied the given initial condition, Equation (3). The set of particular

solutions could be obtained by integrating equation (5) with the following initial values.

$$K_{p,n+1}(0) = 100, \quad c_{p,n+1}(0) = 0 \tag{9}$$

The homogeneous forms of equation (5) were obtained by setting K_n and c_n to zero.

$$\frac{dK_{n+1}(t)}{dt} = K_{n+1}\left(c_n - \frac{2c_nK_n}{N}\right) + c_{n+1}\left(K_n - \frac{(K_n)^2}{N}\right) \tag{10a}$$

$$\frac{dc_{n+1}(t)}{dt} = 0 \tag{10b}$$

The homogeneous solutions could be obtained by integrating equation (10) with the following initial values

$$K_{h1,n+1}(0) = 0$$

$$c_{h1,n+1}(0) = 1 \tag{11}$$

The initial values, equations (9) and (11) were chosen in such a way that at t = 0 the first equation of (6) satisfied condition (4). At t = 0 the following relation could be obtained from the second equation of (6) and the initial values (9) and (11):

$$c_{n+1}(0) = A_{1,n+1} \tag{12a}$$

Since c_{n+1} was a constant function it was evident that relationship (12a)

was true not only for $t = 0$ but also for $0 \leq t \leq t_f$. Therefore,

$$c_{n+1}(t) = A_{1,n+1} \tag{12b}$$

Both the particular and homogeneous solutions were obtained by Runge-Kutta-Gill numerical integration method and the initial values (9) and (11). Therefore, all the terms on the right hand side of Equation (6) were considered as known except $A_{1,n+1}$.

To solve for A_1 the least square functional was used.

$$\theta_{n+1} = \sum_{s=1}^{m_1} \left| K_{n+1}(t)_{CD} - K(t)_{ED} \right|^2 \tag{13a}$$

where m_1 was the number of data points, the CD subscript indicated computed data and the ED subscript indicated generated data.

Substituting equation (6a) into equation (13a),

$$\theta_{n+1} = \sum_{s=1}^{m_1} \left| K_{p,n+1}(t) + A_{1,n+1} K_{h1,n+1}(t) - K(t)_{ED} \right|^2 \tag{13b}$$

The only unknown quantity on the right hand side of equation (13b) was the integration constant, A_1, which was determined by the simplex search technique [Appendix II, Part I]. The objective was to search for the value of A_1, so that the objective function (13b) was minimized. Once the integration constant was known, the general solution of equation (5) could be obtained from equation (6). With K_{n+1} and c_{n+1} known, now an improved set of values could be obtained by making $n = n+1$ in equation (5). The iterative procedure could be continued until the solution converged to the exact parameter with a certain specified accuracy.

2b. NUMERICAL RESULTS

The numerical values used were

$$\Delta t = .05 \quad t_f = 5.0 \quad m_1 = 101$$

The first approximation of K(t) was kept constant at 500. Three different initial approximations c_0 of the parameter c were 6, 10 and 20. It was found that the solution in all three cases converged to the exact value of c which was 2. The influence of the initial approximations, c_0, upon the convergence rate of the constant parameter is shown in Table 2. The convergence rate for the initial approximation of 20 is shown in Figure 1. A computer flow chart for quasilinearization method is shown in Figure 15.

B-3. Numerical Integration and Pattern Search

In this section the constant parameter, c, in equation (1) was identified by the combination of numerical integration and pattern search technique. Any numerical integration scheme and search technique could be used. In this work the Runge-Kutta-Gill computer subroutine [12] and the simplex search technique developed by Nelder and Mead [19] were used, [Appendix II, Part I]. The model was as shown below

$$\frac{dK(t)}{dt} = cK(t)\left[1 - \frac{K(t)}{N}\right] \tag{14}$$

with initial condition

$$K(0) = 100 \tag{15}$$

The classical least squares criterion, shown below, was used as the objective function in the search technique.

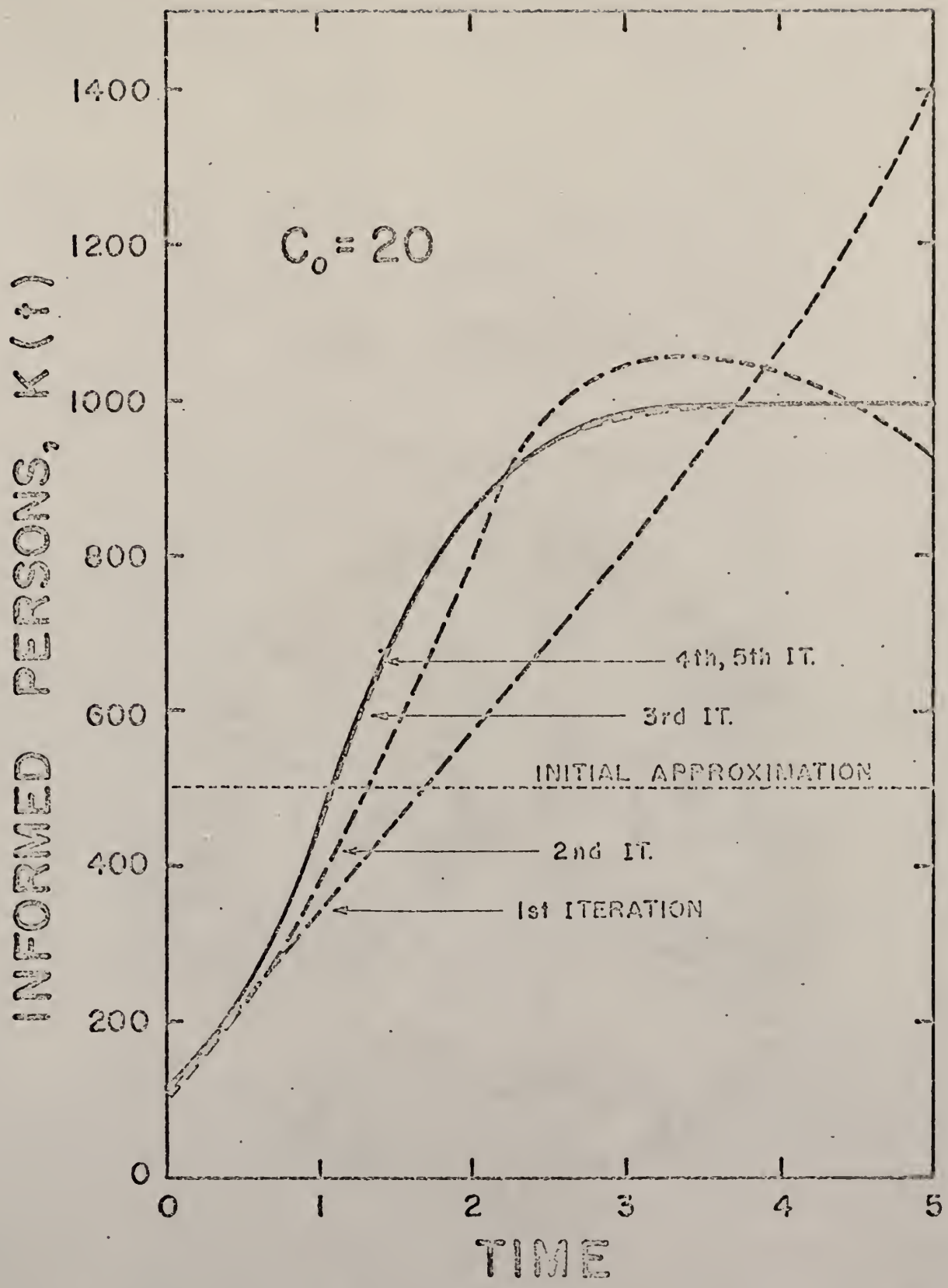

FIGURE 1. CONVERGENCE RATE FOR ONE PARAMETER BY QUASILINEARIZATION.

Table 2. CONVERGENCE RATE OF ONE PARAMETER, QUASILINEARIZATION: WITHOUT NOISE

ITERATION	$C(t_k)$	$C(t_k)$	$C(t_k)$
	6	10	20
1	.9813	.9813	.9813
2	1.7086	1.7086	1.7086
3	1.9710	1.9710	1.9710
4	1.9975	1.9975	1.9975
5	1.9982	1.9982	1.9982
6	1.9982	1.9982	1.9982
TIME IN MINUTES	1.23	1.23	1.23

$$S = Q = \sum_{S=1}^{m_1} \left| K_n(t)_{CD} - K(t)_{ED} \right|^2 \qquad (16)$$

where n denoted the nth evaluation. Each evaluation gave rise to one objective function value.

The objective was to find c so that the square of the difference between the solutions of equation (14) and the experimental data was minimized.

B-3a. Computational Procedure

The problem was composed of equations (14), (15) and (16). With the initial condition of equation (15) and with the first initial approximation of c---p_1 in the search technique---equation (14) was solved by Runge-Kutta-Gill numerical integration. The solutions of equation (14) were substituted into equation (16) to obtain the first value of the objective function, S_1. The process was repeated with a second and third approximations of c---p_2 and p_3 in the search technique---to obtain the second and third values of the objective function, S_2 and S_3. With p_1, p_2 and p_3 a simplex was formed and their respective objective function values were compared. At each simplex p_h, the point with the highest object function value, was replaced by a new point which would be the new approximation of c in equation (14). The whole process was restarted until the parameter c which minimized equation (16) was found. In this case the c found was the exact value of the parameter c. In looking for the new approximation c at each simplex the operations used were reflection, contraction and expansion. (Appendix II, Part I). The new point, p^*, obtained by reflection was

$$p^{*} = 2\bar{p} - p_h \tag{17a}$$

where $\bar{p}$ was the distance from p_h to the mid-point of the line formed by the other two points.

The new point, p^{**}, obtained by contraction was

$$p^{**} = \frac{1}{2} p_h + \frac{1}{2} \bar{p} \tag{17b}$$

The new point, p^{**}, obtained by expansion was

$$p^{**} = 2p^{*} - \bar{p} \tag{17c}$$

B-3b. NUMERICAL RESULTS

The numerical values used were

$$\Delta t = .05 \quad t_f = 5 \quad m_1 = 101$$

Three different first approximations of c were 6, 10 and 20. It was found that the solution in those cases converged to the exact value of c which was 2. The influence of the first approximations of c upon the convergence rate of the constant parameter is shown in Table 3. The convergence rate for the first approximation of 20 is shown in Figure 2. A computer flow chart is shown in Figure 16.

The execution times shown at the end of Table 2 and Table 3 could not be used to conclude that the numerical integration and search method was faster than Quasilinearization. It should be pointed out that within each iteration, search technique was used to solve for the integration constant (Appendix IV, Part I). The time taken to search for the solution of the

Table 3. CONVERGENCE RATE OF ONE PARAMETER, SEARCH AND NUMERICAL INTEGRATION WITHOUT NOISE

EVALUATIONS	$C(t_k)$	$C(t_k)$	$C(t_k)$
0	6.0000	10.0000	20.0000
10	2.0000	3.0000	5.0000
20	2.0000	2.0000	2.0000
30	———	2.0000	2.0000
TIME IN MINUTES	.556	.835	.835

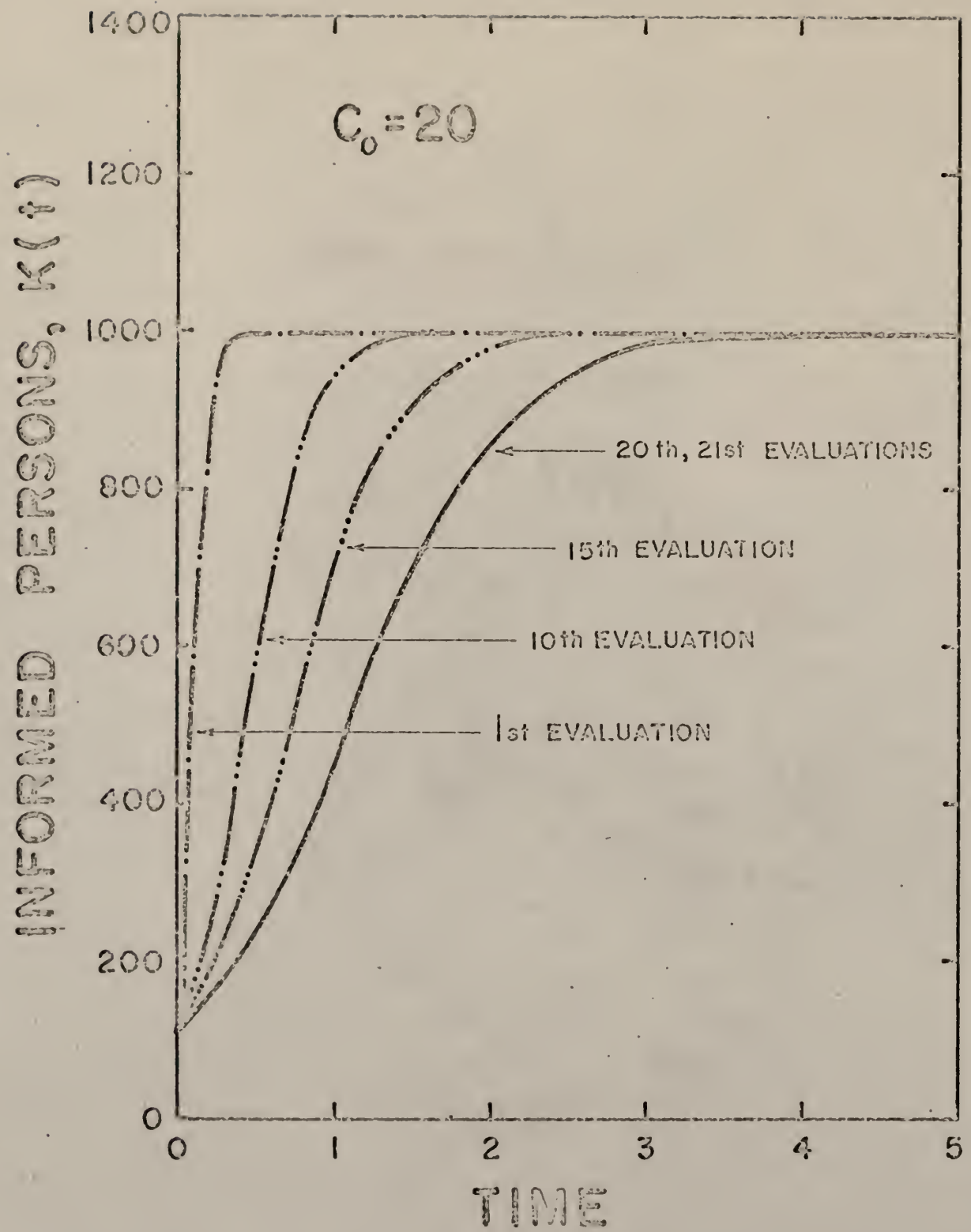

FIGURE 2. CONVERGENCE RATE FOR ONE PARAMETER BY SEARCH AND NUMERICAL INTEGRATION.

integration constant depended very much on the contour of the objective function. Between the first and the sixth iterations the following evaluations were used to solve for the integration constant—55, 201, 50, 35, 29 and 35 giving a total of 405 evaluations. In addition to these evaluations, at each iteration the particular and homogeneous solutions had to be solved yet. Therefore, the time taken for Quasilinearization was more than ten times for the numerical integration and search. If the integration constant were solved by determinant the execution time could be greatly reduced. Based on the fact that it took more than ten times the time to solve for the integration constant in Quasilinearization than for the numerical integration and search method to obtain final solution, it would not be too much of an assumption to say that the former method was ten times faster than the latter.

C. DETERMINISTIC MODEL WITH NOISE

C-1. Experimental data generation

In this section the same parameter c in equation (1) was identified. However, noise was imposed on the experimental data. A normal distribution with a standard deviation of three and a mean of zero of random numbers were generated from an IBM subroutine program [12]. These random numbers were then added to the experimental data without noise as in the following equation

$$K(t)_{wn} = K(t)_{won} + 10 \times R(t) \tag{18}$$

where the subscript wn indicated with noise, won indicated without noise and R(t), random numbers. The random numbers generated are shown in Table 4 and the experimental data with noise obtained are shown in Table 5.

Table 4. RANDOM NUMBERS

NO.	RANDOM NOS.	NO.	RANDOM NOS.	NO.	RANDOM NOS.	NO.	RANDOM NOS.
1	-4.87	2	2.06	3	-3.45	4	3.18
5	-0.25	6	6.20	7	-0.73	8	5.42
9	-2.26	10	1.11	11	-1.38	12	4.59
13	-1.42	14	1.08	15	-4.49	16	2.11
17	-3.97	18	2.41	19	-4.86	20	2.38
21	-2.27	22	0.86	23	-3.94	24	2.70
25	-3.44	26	0.08	27	-5.15	28	0.43
29	-2.54	30	2.58	31	-3.46	32	3.20
33	-5.62	34	4.54	35	-1.80	36	0.88
37	-2.87	38	3.46	39	-1.05	40	2.48
41	-4.28	42	3.99	43	-1.97	44	1.27
45	-3.38	46	2.66	47	-5.69	48	2.74
49	-2.79	50	1.25	51	-2.23	52	3.84
53	-2.16	54	2.69	55	-1.61	56	2.94
57	-3.29	58	1.96	59	-4.90	60	2.14
61	-3.93	62	5.35	63	-0.20	64	2.37
65	-3.71	66	2.88	67	-4.13	68	0.88
69	-1.44	70	1.97	71	-3.58	72	0.79
73	-2.75	74	2.28	75	-2.07	76	1.99
77	-3.43	78	2.13	79	-3.44	80	3.48
81	-3.00	82	2.52	83	-3.37	84	1.62
85	-4.69	86	3.85	87	-2.32	88	1.85
89	-1.43	90	3.80	91	-3.00	92	0.09
93	-1.89	94	1.87	95	-0.57	96	2.28
97	-1.20	98	3.65	99	-3.60	100	1.22
101	-2.64						

Table 5. GENERATED DATA WITH NOISE FOR ONE PARAMETER

TIME	INFORMED PERSONS	TIME	INFORMED PERSONS	TIME	INFORMED PERSONS	TIME	INFORMED PERSONS
0.00	51.30	0.05	130.01	0.10	85.03	0.15	162.23
0.20	139.68	0.25	216.85	0.30	161.07	0.35	237.08
0.40	175.62	0.45	225.68	0.50	218.16	0.55	296.21
0.60	255.28	0.65	300.40	0.70	265.74	0.75	353.49
0.80	315.24	0.85	402.26	0.90	353.33	0.95	450.04
1.00	428.12	1.05	484.27	1.10	461.30	1.15	552.62
1.20	516.10	1.25	574.29	1.30	547.80	1.35	627.43
1.40	620.92	1.45	694.63	1.50	655.93	1.55	743.51
1.60	675.35	1.65	796.13	1.70	751.04	1.75	795.11
1.80	773.88	1.85	852.56	1.90	821.89	1.95	870.72
2.00	815.69	2.05	910.07	2.10	861.36	2.15	903.82
2.20	866.70	2.25	935.70	2.30	860.17	2.35	951.69
2.40	903.12	2.45	949.71	2.50	920.52	2.55	986.39
2.60	931.05	2.65	983.94	2.70	944.84	2.75	993.93
2.80	934.93	2.85	990.41	2.90	924.46	2.95	997.32
3.00	938.87	3.05	1033.73	3.10	980.01	3.15	1007.39
3.20	948.16	3.25	1015.48	3.30	946.55	3.35	997.87
3.40	975.71	3.45	1010.75	3.50	956.02	3.55	1000.48
3.60	965.83	3.65	1016.76	3.70	973.86	3.75	1014.95
3.80	961.24	3.85	1017.19	3.90	961.89	3.95	1031.48
4.00	966.97	4.05	1022.51	4.10	963.82	4.15	1014.01
4.20	951.09	4.25	1036.63	4.30	975.14	4.35	1017.00
4.40	984.30	4.45	1036.78	4.50	968.90	4.55	998.10
4.60	980.16	4.65	1017.87	4.70	1004.99	4.75	1022.17
4.80	987.36	4.85	1035.94	4.90	963.52	4.95	1011.74
5.00	973.15						

The noise on the average was about 3.44% of the data without noise. The noise on the first data point was 48.7% and that on the last data point was 2.64%.

C-2. Quasilinearization

The computation procedure was the same as that in section in B-2 except that in equation (13b), $K(t)_{ED}$ used was the experimental data with noise.

Numerical results

The same numerical values and initial approximations of K(t) and the parameter c were used. Three different initial approximations of c, namely, 6, 10 and 20, the solutions all converged to 1.9783 which was slightly perturbed from the exact parameter of 2 when the generated data without noise was used. 1.9783 was about 3% off from 2. The influence of the initial approximations, c_0 upon the convergence rate of the constant parameter is shown in Table 6 and the convergence rate for the initial approximation of 20 is shown in Figure 3.

C-3. Numerical integration and Pattern Search

The computational procedure was the same as that in Section except that in equation (16), $K(t)_{ED}$ used was the generated data with noise.

Numerical results

The same numerical values and initial approximations of K(t) and the parameter c as that for the data without noise were used. In the three different initial approximations of c namely 6, 10 and 20 the solutions all converged to 22, the exact parameter for the generated data without noise. The convergence rate of the parameter c for the three initial approximations of 6, 10 and 20 were shown in Table 7 and the convergence

Table 6. CONVERGENCE RATE OF ONE PARAMETER, QUASILINEARIZATION WITH NOISE

ITERATION	$C(t_k)$	$C(t_k)$	$C(t_k)$
	6	10	20
1	.9783	.9783	.9783
2	1.6979	1.6979	1.6979
3	1.9545	1.9545	1.9545
4	1.9780	1.9780	1.9780
5	1.9784	1.9784	1.9784
6	1.9783	1.9783	1.9783
7	1.9783	1.9783	1.9783
TIME IN MINUES	1.2100	1.2100	1.2100

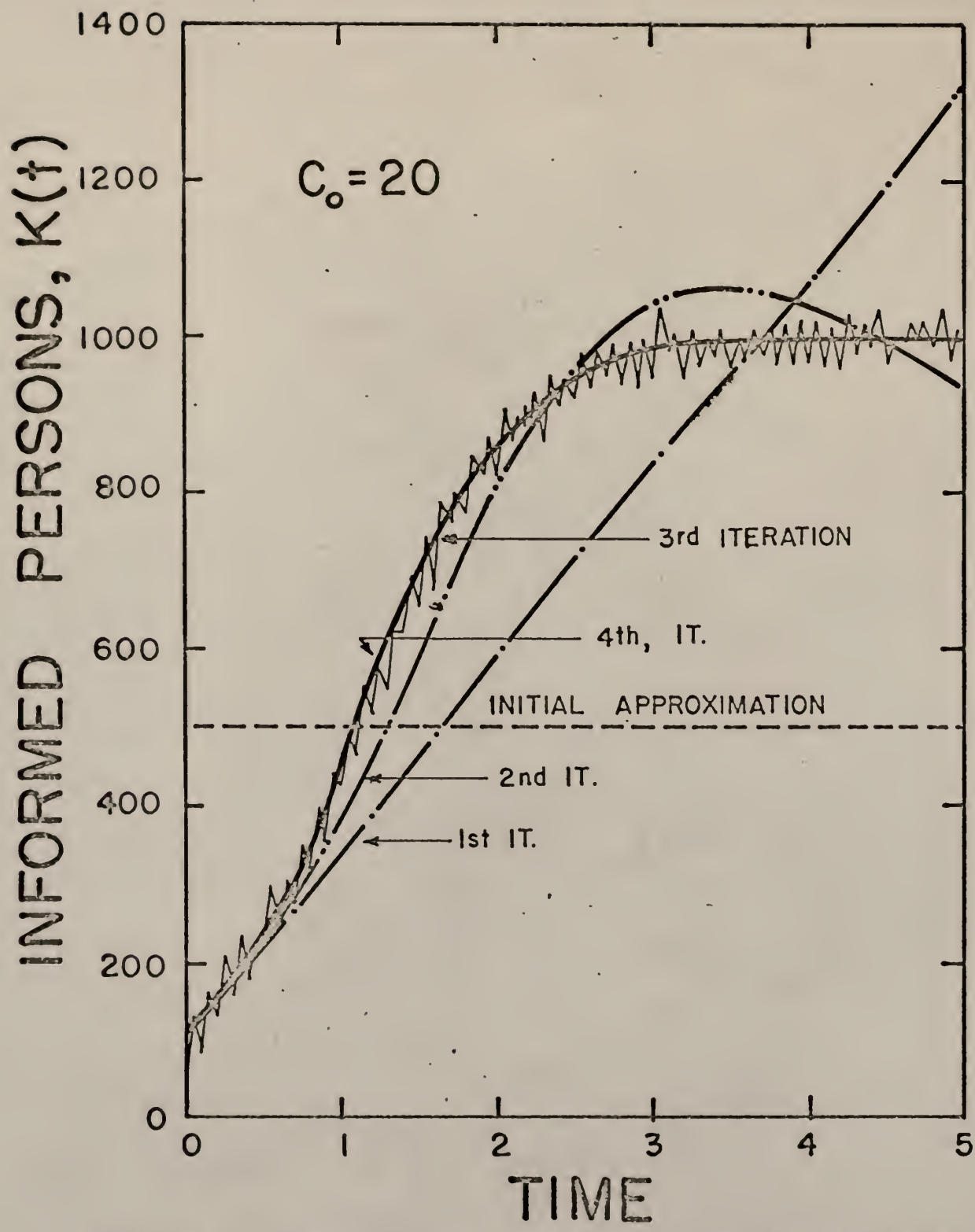

FIGURE 3. CONVERGENCE RATE FOR ONE PARAMETER, WITH NOISE, BY QUASILINEARIZATION.

Table 7. CONVERGENCE RATE OF ONE PARAMETER, SEARCH AND NUMERICAL INTERGRATION WITH NOISE

EVALUATIONS	$C(t_k)$	$C(t_k)$	$C(t_k)$
	6.0000	10.0000	20.0000
10	2.0000	3.0000	5.0000
20	2.0000	2.0000	2.0000
30	———	2.0000	2.0000
-TIME IN MINUTES	0.532	0.7980	0.7980

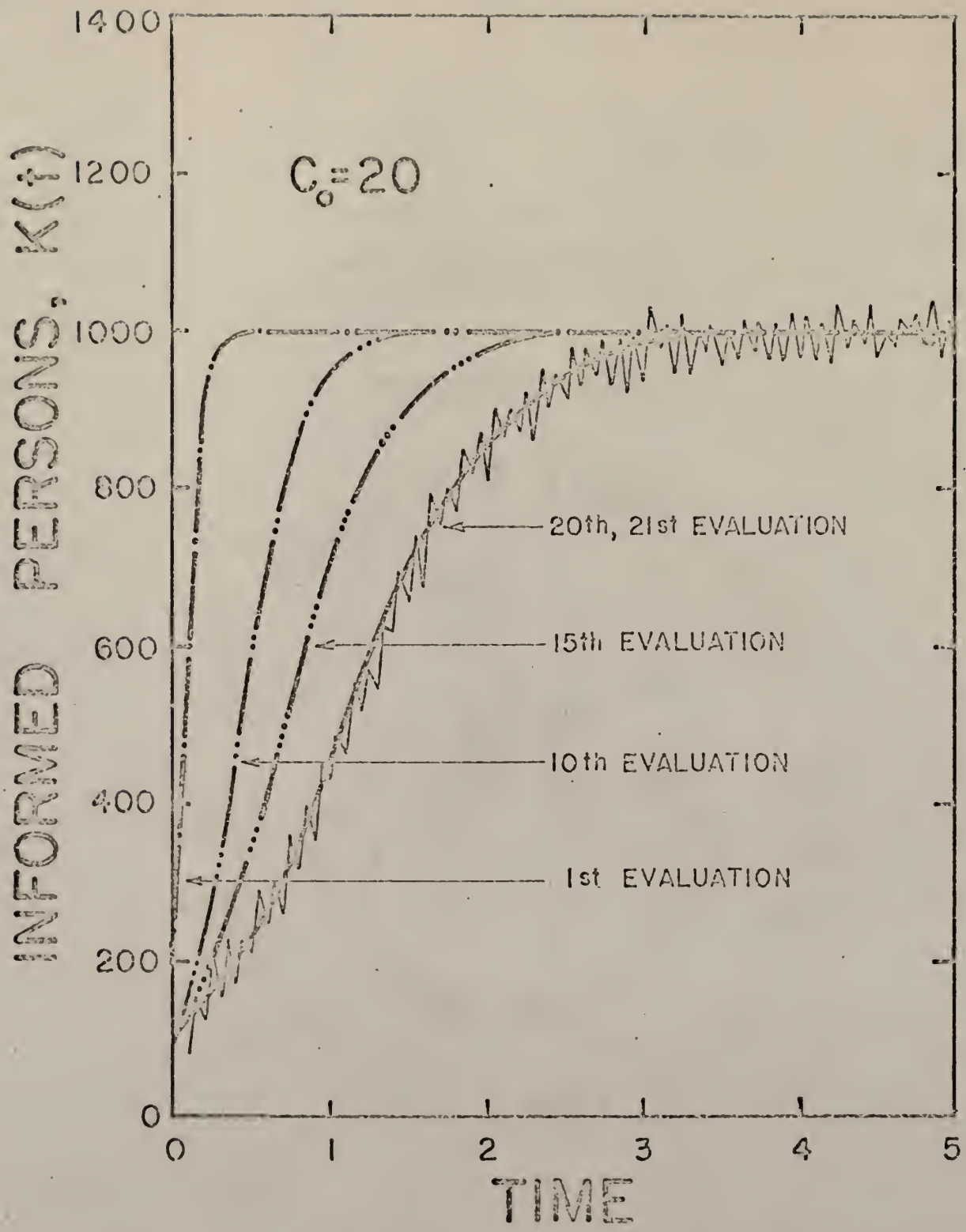

FIGURE 4. CONVEYANCE RATE FOR ONE PARAMETER, WITH NOISE, BY SEARCH AND NUMERICAL INTERGRATION.

rate for an initial approximation of 20 is shown in Figure 4.

Again the times shown at the end of Tables 6 and 7 could not be used as the bases for concluding which method was faster. The same reasing under numerical results in section B-36 of one parameter identification could be applied here. For the seven iterations in Quasilinearization it took altogether 245 evaluations to solve for the integration constants which was about eight times more evaluations for the numerical integration and search method to obtain the final solution.

D. DISCUSSION

Both methods, Quasilinearization and numerical integration and pattern search were successful in identifying one parameter. In the former method the noise had some effect on the solution obtained which was slightly deviated from 2, the exact parameter. However, the initial approximations of c did not have any effect either on the rate of convergence or on the final converged value. In the latter method the noise did not have any effect either on the rate of convergence or on the final converged rate. However, the initial approximations of c had an effect on the rate of convergence. In both method it took just a little bit longer to converge when there was noise in the data.

In Quasilinearization provision was incorporated in the program to terminate the computation at the end of tenth iterations. It termination before ten it was due to an error of too large values for the computer to handle so the machine terminated the computation itself. If less than ten iteration results were presented in a table it was because either the solution converged before tenth iteration or the computer terminated the computation. In either case explanation was given to that effect. If more than ten iterations were shown the program was specially arranged for

a specific purpose.

In the numerical integration and search method the maximum number of evations was limited to two hundred which gave a very accurate result. If less than two two hundred evaluations were presented it meant that the solution was obtained before 200th evaluation.

TWO PARAMETER IDENTIFICATION

As had been shown that both of the methods were successful in identifying the parameter. However, the model used was not very realistic. In this section the model was extended to make it more practical and two parameters were identified. The same two methods were used. Again the data used was first without noise and then with noise.

A. The Model

The model [23] used here was an extended one of one parameter. The total number of members in the group was no longer considered as constant but growing with time. At the same time when the total number was growing some of the informed members were removed from the group. The differential equation now became

$$\frac{dK(t)}{dt} = cK(t)\left|1 - \frac{K(t)}{N_0 e^{gt}}\right| - \gamma K(t) \qquad (19)$$

where

N_0 = number of members in the group at $t = 0$

g = rate at which new members were added to the group

γ = rate at which members were removed from the group

c = contact coefficient

$cK(t)$ = number of contacts made in the time interval dt

e^{gt} = growth factor

$N_0 e^{gt}$ = number of members at time t.

$\gamma K(t)$ = informed persons removed from the group in time dt

$\frac{dK(t)}{dt}$ = increase in the number of informed persons

In addition to parameter c, parameter γ was also identified. γ was the rate at which the informed persons were removed from the group. This parameter differed from group to group and also from location to location. It had an indirect effect on the means and frequency of advertising which was dictated by the contact coefficient c as mentioned earlier under one parameter identification. For a certain desired number of informed persons in the group the contact coefficient was directly proportional to the removal coefficient.

B. Deterministic Model Without Noise

B-1. Experimental Data Generation

The experimental data was generated by actually solving equation (19) with Runge-Kutta-Gill Numerical integration technique

The following constants and step size were used

$K(0)$ = 50 informed persons at t = 0

N_0 = 100 members in the group at t = 0

Table 8. GENERATED DATA WITHOUT NOISE FOR TWO AND THREE PARAMETERS

TIME	INFORMED PERSONS	TIME	INFORMED PERSONS	TIME	INFORMED PERSONS	TIME	INFORMED PERSONS
0.000	50.00	0.025	51.24	0.050	52.45	0.075	53.64
0.100	54.80	0.125	55.94	0.150	57.06	0.175	58.16
0.200	59.23	0.225	60.29	0.250	61.32	0.275	62.34
0.300	63.35	0.325	64.34	0.350	65.31	0.375	66.27
0.400	67.22	0.425	68.17	0.450	69.10	0.475	70.02
0.500	70.94	0.525	71.85	0.550	72.76	0.575	73.66
0.600	74.55	0.625	75.45	0.650	76.34	0.675	77.24
0.700	78.13	0.725	79.02	0.750	79.92	0.775	80.81
0.800	81.71	0.825	82.61	0.850	83.51	0.875	84.42
0.900	85.33	0.925	86.25	0.950	87.17	0.975	88.09
1.000	89.02	1.025	89.96	1.050	90.90	1.075	91.85
1.100	92.80	1.125	93.77	1.150	94.74	1.175	95.72
1.200	96.71	1.225	97.70	1.250	98.70	1.275	99.71
1.300	100.73	1.325	101.76	1.350	102.80	1.375	103.85
1.400	104.90	1.425	105.97	1.450	107.05	1.475	108.13
1.500	109.23	1.525	110.33	1.550	111.45	1.575	112.58
1.600	113.72	1.625	114.87	1.650	116.03	1.675	117.20
1.700	118.38	1.725	119.57	1.750	120.78	1.775	122.00
1.800	123.23	1.825	124.47	1.850	125.72	1.875	126.99
1.900	128.27	1.925	129.56	1.950	130.86	1.975	132.18
2.000	133.51	2.025	134.85	2.050	136.21	2.075	137.58
2.100	138.97	2.125	140.36	2.150	141.78	2.175	143.20
2.200	144.64	2.225	146.10	2.250	147.57	2.275	149.05
2.300	150.55	2.325	152.06	2.350	153.59	2.375	155.14
2.400	156.69	2.425	158.27	2.450	159.86	2.475	161.47
2.500	163.09						

The least square criteria shown below was used to determine the parameters c and γ so that the sum of the squares of the deviations was minimized.

$$Q = \sum_{S=1}^{m_1} \left| x(t_S) - b_S \right|^2 \tag{21}$$

Systems (19) and (20) were treated as a multipoint boundary-value problem.

B-2a. Computational Procedure

The parameter identification problem by Quasilinearization was composed of equation (19), (20) and (21).

The recurrence relation for the system of equations (19) could be obtained from equation (10) in Appendix I, Part I:

$$\frac{dK_{n+1}(t)}{dt} = c_n K_n \left| 1 - \frac{K_n}{N_0 e^{gt}} \right| - \gamma_n K_n$$

$$+ (K_{n+1} - K_n) \left| c_n - \frac{2c_n K_n}{N_0 e^{gt}} \right| - \gamma_n$$

$$+ (c_{n+1} - c_n) \left| K_n - \frac{(K_n)}{N_0 e^{gt}} \right|$$

$$+ (\gamma_{n+1} - \gamma_n)(-K_n) \tag{22a}$$

$g = .4$

γ = 2 persons removed per unit time

c = 6 persons contacted per unit time

$t(0) = 0$ initial time.

$t_f = 2.5$ final time

$\Delta t = .025$ integration step size

The relationship between time t and the informed person K(t) was shown in Table 8.

B-2. Quasilinearization

The two constant parameters c and γ were identified by Quasilinearization and the least square criterion. The model was shown again as below

$$\frac{dK(t)}{dt} = cK(t)\left|1 - \frac{K(t)}{N_0 e^{gt}}\right| - \gamma K(t) \tag{19a}$$

Again the two unknown parameters c and γ were treated as dependent variables and as functions of the independent variable t. In addition to equation (19a) the two constant unknown parameters could be represented by the following differential equations [16]:

$$\frac{dc}{dt} = 0 \tag{19b}$$

$$\frac{d\gamma}{dt} = 0 \tag{19c}$$

The initial condition for equation (19a) was

$$K(0) = 50 \tag{20}$$

$$\frac{dc_{n+1}(t)}{dt} = 0 \tag{22b}$$

$$\frac{d\gamma_{n+1}(t)}{dt} = 0 \tag{22c}$$

where the subscript n represented the nth iteration.

In equations (22) K_{n+1}, c_{n+1} and γ_{n+1} were considered as unknown functions of t and K_n, c_n and γ_n were considered as know functions of t obtained from the (n-1)st iterative solution. The above three equations became three simultaneous first order linear differential equations. The general solutions for the above three equations were obtained by superposition principle [16]. With one initial condition (20) given, only two sets of homogeneous solutions were needed for the three equation in (22). Thus, the general solutions of equation (22) were:

$$K_{n+1}(t) = K_{p,n+1}(t) + \sum_{j=1}^{2} A_{j,n+1} K_{hj,n+1}(t) \tag{23a}$$

$$c_{n+1}(t) = c_{p,n+1}(t) + \sum_{j=1}^{2} A_{j,n+1} c_{hj,n+1}(t) \tag{23b}$$

$$\gamma_{n+1}(t) = \gamma_{p,n+1}(t) + \sum_{j=1}^{2} A_{j,n+1} \gamma_{hj,n+1}(t) \tag{23c}$$

Subscript p indicated particular solutions and h_1 and h_2 denoted the first and second sets of homogeneous solutions respectively. $A_{1,n+1}$ and $A_{2,n+1}$ were integration constants to be determined from simplex search technique. Equation (23) could be written in matrix form:.

$$K_{n+1}(t) = K_{p(n+1)}(t) + K_{h(n+1}(t)A_{n+1} \tag{24}$$

where $K_{n+1}(t)$ and $K_{p(n+1)}(t)$ were defined as

$$K_{n+1}(t) = \begin{vmatrix} K_{n+1}(t) \\ c_{n+1}(t) \\ \gamma_{n+1}(t) \end{vmatrix}, \quad K_{p(n+1)}(t) = \begin{vmatrix} K_{p,n+1}(t) \\ c_{p,n+1}(t) \\ \gamma_{p,n+1}(t) \end{vmatrix} \tag{25}$$

The homogeneous matrix was defined as

$$K_{h(n+1)}(t) = \begin{vmatrix} K_{h1,n+1}(t) & K_{h2,n+1}(t) \\ c_{h1,n+1}(t) & c_{h2,n+1}(t) \\ \gamma_{h1,n+1}(t) & \gamma_{h2,n+1}(t) \end{vmatrix} \tag{26}$$

and A_{n+1} represented the integration constant vector with components $A_{1,n+1}$ and $A_{2,n+1}$. The particular and homogeneous solutions were chosen so that they satisfied the given initial condition, Equation (20). The set of particular solutions could be obtained by integrating equation (22) with the following initial values.

$$K_{p,n+1}(0) = 50, \quad c_{p,n+1}(0) = 0, \quad \gamma_{p,n+1}(0) = 0 \tag{27}$$

The homogeneous forms of equation (22) were:

$$\frac{dK_{n+1}(t)}{dt} = K_{n+1}\left|c_n - \frac{2c_nK_n}{N_0e^{gt}}\right| - \gamma_n$$

$$+ c_{n+1}\left|K_n - \frac{(K_n)^2}{N_0e^{gt}}\right|$$

$$+ \gamma_{n+1}(-K_n), \tag{28a}$$

$$\frac{dc_{n+1}(t)}{dt} = 0 \tag{28b}$$

$$\frac{d\gamma_{n+1}(t)}{dt} = 0 \tag{28c}$$

The homogeneous solutions could be obtained by integrating equation (28) with the following initial values.

$$K_{h(n+1)}(t) = \begin{vmatrix} 0 & 0 \\ 1 & 0 \\ 0 & 1 \end{vmatrix} \tag{29}$$

The initial values (27) and (29) were chosen so that at t = 0 equation (23) satisfied Equation (20). At t = 0 the following two relationships could be obtained from equations (23b), (23c), and the initial values of (27) and (29).

$$c_{n+1}(0) = A_{1,n+1},\ \gamma_{n+1}(0) = A_{2,n+1} \tag{30}$$

Since c_{n+1} and γ_{n+1} were constant functions, it was evident that relationships Equation (30) was true for $0 \leq t \leq t_f$. Therefore,

$$c_{n+1}(t) = A_{1,n+1},\ \gamma_{n+1}(t) = A_{2,n+1}$$

Both the particular and homogeneous solutions were considered as known because they were obtained by RKGS method with the initial values of (27) and (29). Therefore, in the right hand side of equation (23) only the integration constants $A_{1,n+1}$ and $A_{2,n+1}$ were unknown and they were determined by the simplex search technique.

The least square criterion

$$Q_{n+1} = \sum_{s=1}^{m_1} \Big| K_{p,n+1}(t) + A_{1,n+1}\, K_{h1,n+1}(t) + A_{2,n+1}\, K_{h2,n+1}(t) - K(t)_{ED} \Big|^2 \qquad (31)$$

became the objective function in the search. Once the integration constants became known, the general solution of equation (22) could be obtained from equation (23). With K_{n+1}, c_{n+1} and γ_{n+1} known an improved set of values could be obtained by making n = n+1 in equation (22). The iteration was continued until the solution converged to the exact parameter with a certain desired accuracy.

B-2b. NUMERICAL RESULTS

The numerical values used were

$$\Delta t = .025 \quad t_f = 2.5 \quad m_1 = 101$$

The first approximation of K(t) was kept constant at .80 for the first iteration. The exact parameter values of $c(t_K) = 6$ and $\gamma(t_K) = 2$

were used as the initial approximations. The solution did not converge at the end of ten iterations. The values of the parameters for each of the ten iterations are shown in Table 9A and the curve fitting is shown in Figure 5.

A few attempts were made to help the solution to converge.

1. The first approximation of K(t) was kept constant at 60 throughout the first iteration. The results are shown in Table 9B. At fourth iteration the numerical solution of the model approached infinity.
2. The first approximation of K(t) was then kept constant at 150 throughout the first iteration. The results are shown in Table 9C. At third iteration the numerical solution of the model approached infinity.
3. In the search for the solution of c and γ at each iteration by the simplex technique the following constraints were imposed on the parameters

$$1 < c(t_K) < 10.5$$

$$.5 < \gamma(t_K) < 4$$

The two parameters seemed to oscillate and at the fifth iteration while solving for the integration constants by the search technique the program was stopped because in subroutine Scheck (Appendix IV, Part I) the sum of the square of the difference between the objective function and the mean of the three objective functions in a simplex approached infinity. Results up to fourth iteration are shown in Table 9D.

Table 9A. CONVERGENCE RATE OF TWO PARAMETERS, QUASILINEARIZATION WITHOUT NOISE

ITERATIONS	$C(t_k)$	$\gamma(t_k)$
0	6.0000	2.0000
1	-1.5654	4.1859
2	-1.8967	2.9106
3	3.0752	-5.1375
4	3.6031	-2.8323
5	4.1605	-2.7274
6	4.2205	-2.7249
7	4.2331	-2.7317
8	4.2347	-2.7354
9	4.2331	-2.7358
10	4.2325	-2.7356

Time = 5.10 minutes

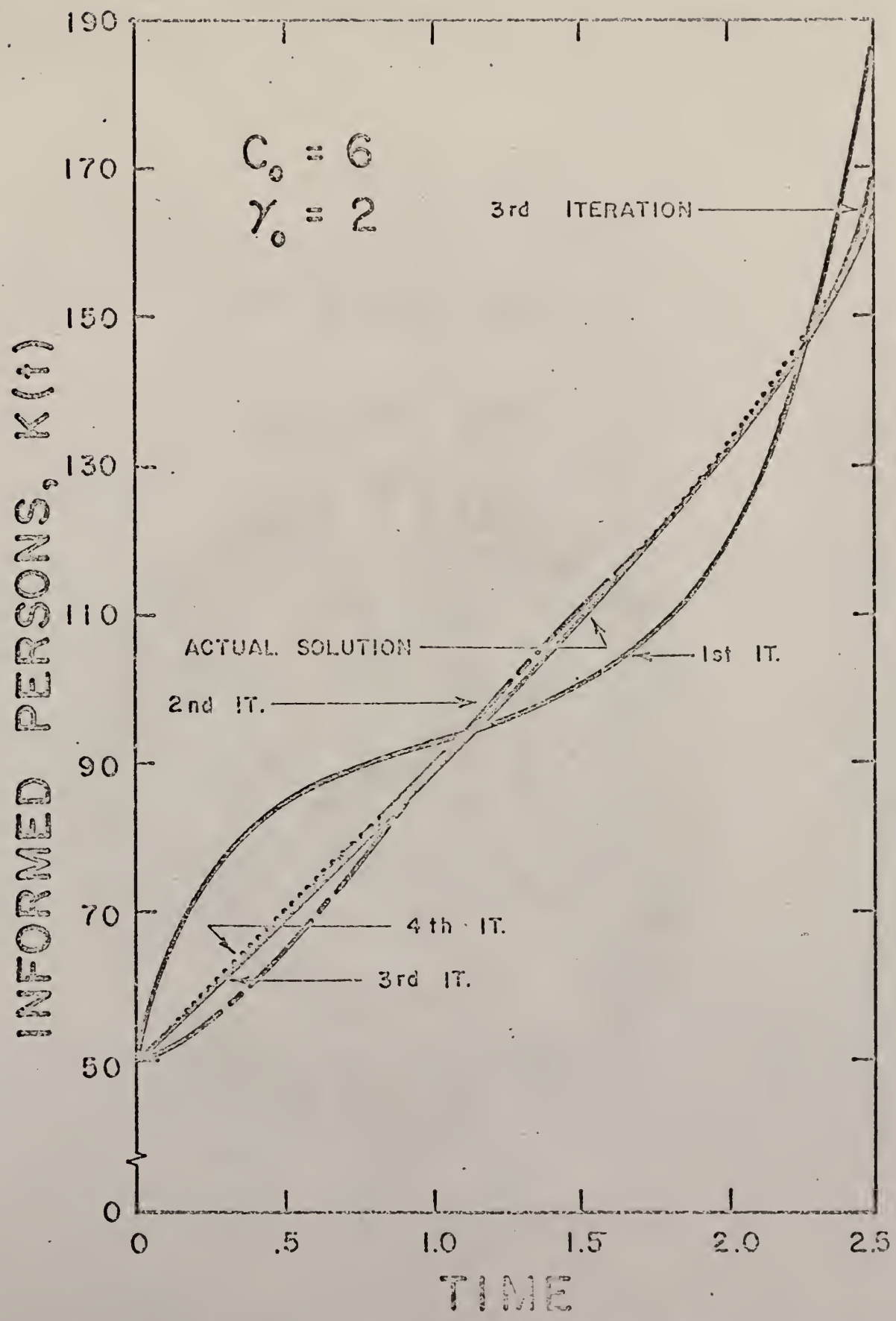

FIGURE 5. CONVERGENCE RATE FOR TWO PARAMETERS BY QUASILINEARIZATION.

4. On examination of Figure 5. It was noticed that at each iteration the solution approached the actual solution, yet it was not stable. To stabilize the solution, perturbation was used. The first formula used was as shown below

$$K(1)_n = K(0)_{n+1} + \alpha(b_S - K(0)_{n+1})$$

$K(1)_n = K_n$ for the next iteration

$K(0)_{n+1}$ = the solution obtained at present iteration

α = perturbation factor which could be from 0 to 1.

The results are shown in Table 9E where the value of alpha used was .2. The solution seemed to converge to 4.25 for c and -2.76 for γ.

5. The above formula was used again but alpha was set to .05. The results are shown in Table 9F. The number of iterations were extended to 20 instead of 10. The solution converged to 4.24 for c and -2.74 for γ.

6. Trials 4 and 5 seemed to have stabilized the solution which converged to 4.24 for c and -2.74 for γ. To improve the solution constraints was imposed on the parameters.

   The same constraints used in trial 3 was used here. The results are shown in Table 9G. The solution again seemed to oscillate once the constraints were imposed.

7. The next attempt was to use a different perturbation as shown below

$$K(1)_n = K(0)_n + \alpha(K(0)_{n+1} - K(0)_n)$$

$K(1)_n = K_n$ for the next iteration

$K(0)_{n+1}$ = solution of present iteration

$K(0)_n = K_n$ of present iteration

$0 < \alpha < 1$

Two values of alpha used were .1 and .4. The results are shown in Tables 9H and 9I. The solutions for $\alpha = .1$ were unstable and oscillated at the end of ten iterations. To study the effect of α, the value was increased to .4 and iterations extended to 18. It was observed that by increasing α it became stable faster. The solution for the latter case seemed to converge to 4.23 for c and -2.73 for γ. In all the above seven attempts the exact parameters were used as the first approximations.

B-3. Numerical Integration and Pattern Search

The same two parameters c and γ of equation (19a) were identified by numerical integration and pattern search. In this work the Runge-Kutta-Gill [12] computer subroutine and the simplex search technique [20] were used. The methods were discussed in the Appendia II and III, Part I. The model was reproduced below.

$$\frac{dK(t)}{dt} = cK(t)\left[1 - \frac{K(t)}{N_0 e^{gt}}\right] - \gamma K(t) \qquad (32)$$

with initial condition

Table 9B. CONVERGENCE RATE OF TWO PARAMETERS, QUASILINEARIZATION WITHOUT NOISE

$K(0) = 60$

ITERATIONS	$C(t_k)$	$\gamma(t_k)$
0	6.0000	2.0000
1	-10.9673	28.7084
2	-28.7610	30.2639
3	-28.8992	30.4466

Time = 2.42 minutes

Table 9C. CONVERGENCE RATE OF TWO PARAMETERS, QUASILINEARIZATION WITHOUT NOISE

$K(0) = 150$

ITERATIONS	$C(t_k)$	$\gamma(t_k)$
0	6.0000	2.0000
1	-20.7555	55.3068
2	-56.0861	57.6009

Time = 1.70 minutes

Table 9D. CONVERGENCE RATE OF TWO PARAMETERS WITH CONSTRAINTS, QUASI-LINEARIZATION WITHOUT NOISE

CONSTRAINTS: $1 < C(t_k) < 10.5$

$.5 < \gamma(t_k) < 4$

ITERATIONS	$C(t_k)$	$\gamma(t_k)$
0	6.0000	2.0000
1	1.0000	0.5001
2	1.9583	2.0357
3	1.0000	0.5000
4	1.9044	2.0465

Time = 3.01 minutes

Table 9E. CONVERGENCE RATE OF TWO PARAMETERS WITH PERTURBATION, QUASILINEARIZATION WITHOUT NOISE

$$K(1)_n = K(0)_{n+1} + \alpha\,(b_s - K(0)_{n+1})$$

$$\alpha = .2$$

ITERATIONS	$C(t_k)$	$\gamma(t_k)$
0	6.0000	2.0000
1	-1.5654	4.1859
2	-1.8967	2.9106
3	3.2470	-5.4378
4	3.6264	-2.8859
5	4.1730	-2.7550
6	4.2479	-2.7527
7	4.2559	-2.7568
8	4.2580	-2.7598
9	4.2571	-2.7603
10	4.2563	-2.7601

Time = 5.65 minutes

Table 9F. CONVERGENCE RATE OF TWO PARAMETERS WITH PERTURBATION, QUASILINEARIZATION WITHOUT NOISE

$$K(1)_n = K(0)_{n+1} + \alpha\ (b_s - K(0)_{n+1})$$

$$\alpha = .05$$

ITERATIONS	$C(t_k)$	$\gamma(t_k)$
0	6.000	2.0000
1	-1.5652	4.1854
2	-1.8966	2.9108
3	3.1133	-5.2039
4	3.6084	-2.8445
5	4.1629	-2.7335
6	4.2296	-2.7329
7	4.2410	-2.7397
8	4.2440	-2.7443
9	4.2409	-2.7442
10	4.2391	-2.7430
11	4.2392	-2.7426
12	4.2394	-2.7426
13	4.2405	-2.7432
14	4.2403	-2.7434
15	4.2391	-2.7427
16	4.2395	-2.7427
17	4.2425	-2.7446
18	4.2397	-2.7436
19	4.2383	-2.7423
20	4.2410	-2.7435

TIME IN MINUTES = 9.09

Table 9G. CONVERGENCE RATE OF TWO PARAMETERS WITH PERTURBATION, QUASILINEARIZATION WITHOUT NOISE

$$K(1)_n = K(0)_{n+1} + \alpha\ (b_s - K(0)_{n+1})$$

$$\alpha = .1$$

CONSTRAINTS: $1 < C(t_k) < 10.5$

$$.5 < \gamma(t_k) < 4$$

ITERATIONS	$C(t_k)$	$\gamma(t_k)$
0	6.0000	2.0000
1	1.0000	0.5001
2	1.9515	2.0527
3	1.0000	0.5000
4	1.8971	2.0516
5	1.0001	0.5009
6	1.8973	2.0587
7	1.0000	0.5000
8	1.8973	2.0513
9	1.0000	0.5000
10	1.8970	2.0514

Time = 5.45 minutes

Table 9H. CONVERGENCE RATE OF TWO PARAMETERS WITH PERTURBATION, QUASILINEARIZATION WITHOUT NOISE

$$K(1)_n = K(0)_n + \alpha(K(0)_{n+1} - K(0)_n)$$

$$\alpha = .1$$

ITERATIONS	$C(t_k)$	$\gamma(t_k)$
0	6.0000	2.0000
1	-1.5654	4.1859
2	-1.8967	2.9106
3	-2.4465	4.5489
4	-3.4206	4.9496
5	-4.9771	6.9203
6	-7.4502	9.3544
7	-4.6802	5.5692
8	5.4370	-7.0235
9	2.9927	-2.5073
10	4.8869	-3.0169

TIME = 6.35 MINUTES

Table 9I. CONVERGENCE RATE OF TWO PARAMETERS WITH PERTURBATION, QUASILINEARIZATION WITHOUT NOISE

$$K(1)_n = K(0)_n + \alpha\ (K(0)_{n+1} - K(0)_n)$$

$$\alpha = .4$$

ITERATIONS	$C(t_k)$	$\gamma(t_k)$
0	6.0000	2.0000
1	-1.5652	4.1854
2	-1.8966	2.9108
3	-3.5131	6.4285
4	7.7529	-9.7123
5	3.2430	-2.8448
6	4.7092	-3.0745
7	4.3930	-2.9622
8	4.3114	-2.8702
9	4.2706	-2.8107
10	4.2515	-2.7764
11	4.2423	-2.7575
12	4.2374	-2.7472
13	4.2322	-2.7399
14	4.2340	-2.7382
15	4.2332	-2.7370
16	4.2342	-2.7371
17	4.2345	-2.7374
18	4.2340	-2.7372

Time = 10.16 minutes

$$K(0) = 50 \tag{33}$$

The classical least squares criterion, shown below, was used as the objective function in the search technique

$$S = Q = \sum_{S=1}^{m_1} \left| K_n(t)_{CD} - K(t)_{ED} \right|^2 \tag{34}$$

The objective was to find c and γ so that the sum of the square of deviations between the solution of equation (32) and the generated data was minimized.

B-3a. Computation Procedure

The problem was composed of equations (32), (33) and (34). With the initial condition of equation (33) and with the first initial approximation of c and γ (two dimensional search) — p_1 in the search technique (Appendix II, Part I) — equation (32) was solved by Runge-Kutta-Gill numerical integration (Appendix III, Part I). The solutions of equation (32) were substituted into equation (34) to obtain the first value of the objective function S_1. This process was repeated with a second and third approximations of c and γ — p_2 and p_3 in the search technique — to obtain the second and third values of the objective function, S_2 and S_3. With p_1, p_2 and p_3 a simplex was formed and their respective objective function values were compared. At each simplex p_h, the point with the highest objective function values, was replaced by a new point which would be the new approximation of c and γ in equation (32). In looking for the new points Equations (17a) through (c) under one parameter identification were used. The whole process was repeated until the solution converged to c and γ.

B-3b. NUMERICAL RESULTS

The numerical values used were

$$\Delta t = .025 \quad t_f = 2.5 \quad m_1 = 101$$

Two different sets of initial approximations of c and γ were used, namely 1; .2 and 12; 5. They were chosen arbitrarily. It was found that the solution in two cases converged to the exact values 6 and 2 of the parameters c and γ. The influence of the first approximations of c and γ upon the convergence rate of the constant parameters is shown in Table 10 and the convergence rate for the first approximation of $c_0 = 1$, $\gamma_0 = .2$ and $c_0 = 12$; $\gamma_0 = 5$ shown in Figures 6 and 7, respectively.

C. Deterministic model with noise

C-1. Experimental data generation

The same parameters c and γ of the model (19a) were identified. However, noise was imposed on the generated data in the same manner as in section c - 1 under the one parameter and as shown below in Equation (34a). The generated data with noise are shown in Table 11. The noise on the average was about 2.55% of the data without noise. The noise imposed on the first and last generated data was about 9.74% and 1.62% respectively.

$$K(t)_{wn} = K(t)_{won} + R(t)$$

C-2. Quasilinearization

Computational Procedure

The computational procedure was the same as in Section B-2 of the

Table 10. CONVERGENCE RATE OF TWO PARAMETERS, SEARCH AND NUMERICAL INTEGRATION WITHOUT NOISE

EVALUATIONS	$C(t_k)$	$\gamma(t_k)$	$C(t_k)$	$\gamma(t_k)$
1	1.0000	0.2000	12.0000	5.0000
10	1.7000	0.2000	12.7000	4.7000
20	1.9690	0.3485	12.5845	4.6525
30	3.5762	1.0271	11.9553	4.4190
40	5.9092	1.9677	5.1582	1.6561
50	6.0797	2.0335	5.7832	1.9132
60	5.9754	1.9899	6.0830	2.0330
70	5.9957	1.9982	6.0179	2.0072
80	5.9995	1.9998	6.0024	2.0010
90	5.9998	1.9999	6.0005	2.0002
100	5.9999	1.9999	5.9999	1.9999
TIME IN MINUTES	3.5		3.5	

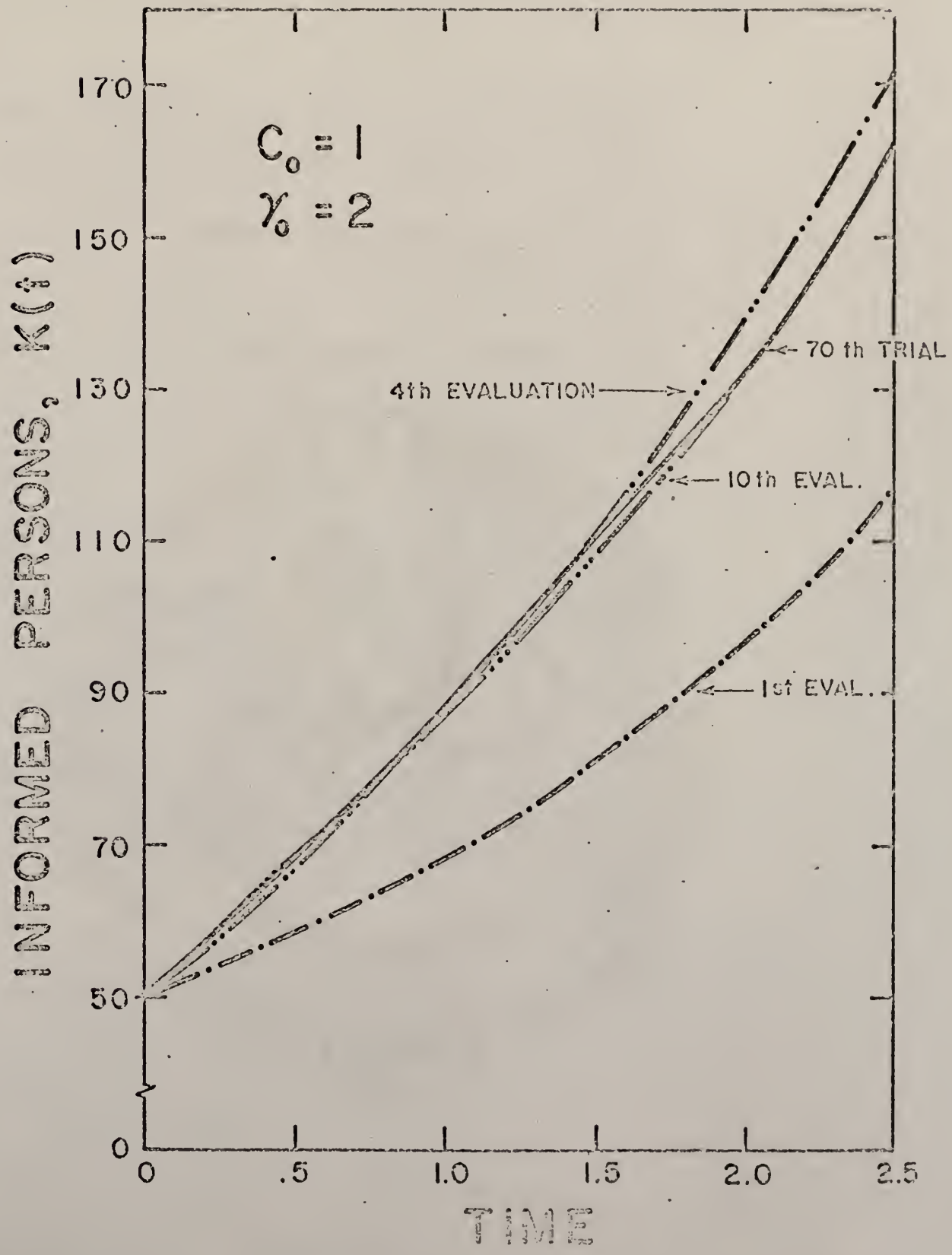

FIGURE 6. CONVERGENCE RATE FOR TWO PARAMETERS BY SEARCH AND NUMERICAL INTEGRATION.

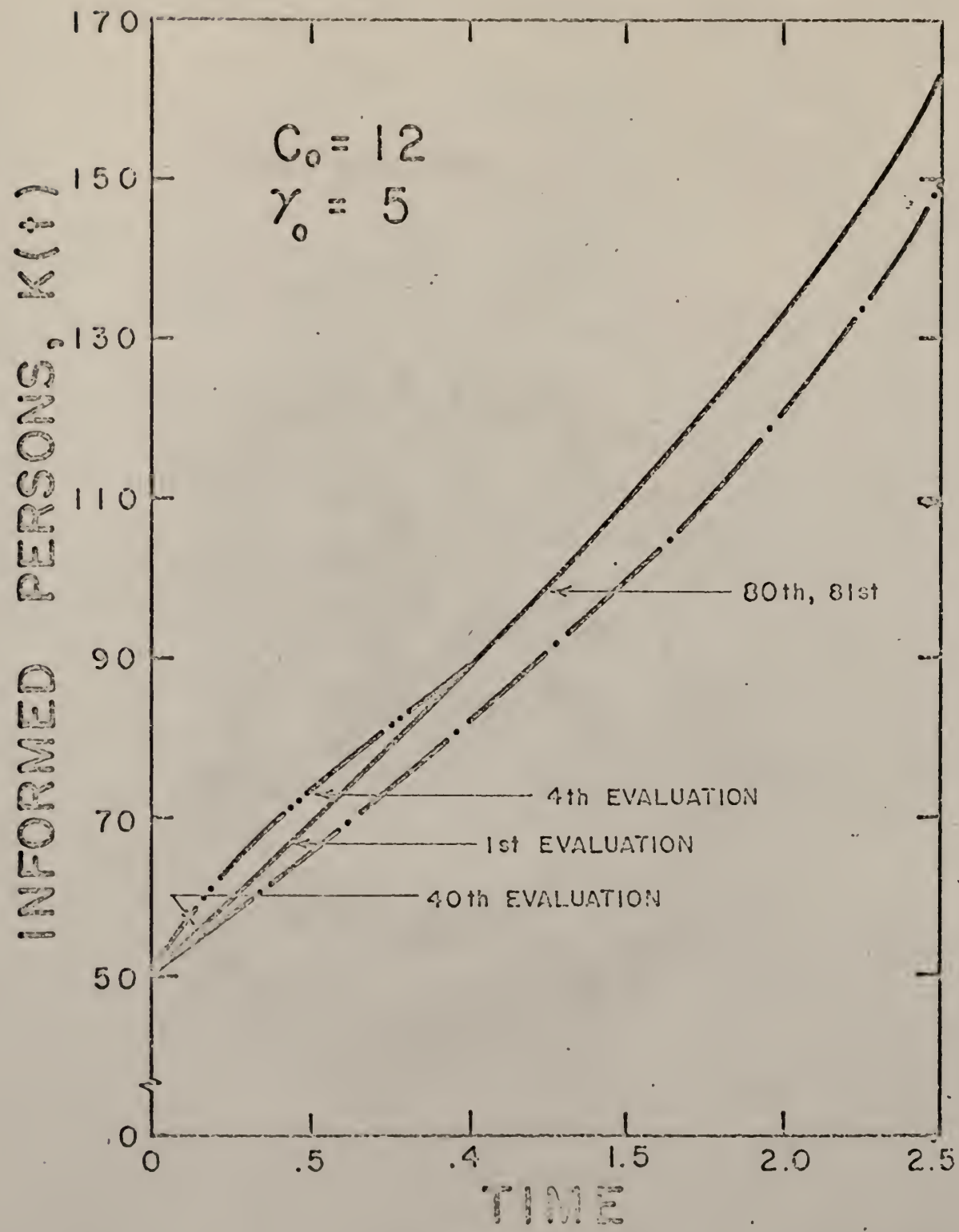

FIGURE 7. CONVERGENCE RATE FOR TWO PARAMETERS BY SEARCH AND NUMERICAL INTEGRATION.

Table 11.GENERATED DATA WITH NOISE FOR TWO AND THREE PARAMETERS

TIME	INFORMED PERSONS	TIME	INFORMED PERSONS	TIME	INFORMED PERSONS	TIME	INFORMED PERSONS
0.000	45.13	0.025	53.30	0.050	49.00	0.075	56.82
0.100	54.55	0.125	62.14	0.150	56.33	0.175	63.58
0.200	56.97	0.225	61.39	0.250	59.94	0.275	66.94
0.300	61.93	0.325	65.41	0.350	60.82	0.375	68.38
0.400	63.25	0.425	70.57	0.450	64.23	0.475	72.40
0.500	68.67	0.525	72.71	0.550	68.82	0.575	76.35
0.600	71.11	0.625	75.37	0.650	71.19	0.675	77.67
0.700	75.59	0.725	81.61	0.750	76.45	0.775	84.01
0.800	76.09	0.825	87.15	0.850	81.72	0.875	85.30
0.900	82.46	0.925	89.70	0.950	86.12	0.975	90.57
1.000	84.74	1.025	93.95	1.050	88.93	1.075	93.12
1.100	89.43	1.125	96.43	1.150	89.06	1.175	98.46
1.200	93.92	1.225	98.95	1.250	96.47	1.275	103.56
1.300	98.57	1.325	104.46	1.350	101.19	1.375	106.79
1.400	101.62	1.425	107.93	1.450	102.15	1.475	110.27
1.500	105.30	1.525	115.69	1.550	111.25	1.575	114.94
1.600	110.01	1.625	117.75	1.650	111.89	1.675	118.08
1.700	116.94	1.725	121.55	1.750	117.20	1.775	122.78
1.800	120.48	1.825	126.75	1.850	123.66	1.875	128.98
1.900	124.84	1.925	131.69	1.950	127.42	1.975	135.66
2.000	130.51	2.025	137.38	2.050	132.84	2.075	139.21
2.100	134.28	2.125	144.21	2.150	139.46	2.175	145.05
2.200	143.21	2.225	149.90	2.250	144.57	2.275	148.96
2.300	148.66	2.325	153.94	2.350	154.16	2.375	157.42
2.400	155.49	2.425	161.92	2.450	156.26	2.475	162.69
2.500	160.45						

parameter identification except that in equation (31), $K(t)_{ED}$ used was the generated data with noise.

Numerical Results

The numerical values used were

$$\Delta t = .025 \quad t_f = 2.5 \quad m_1 = 101$$

The first approximation of K(t) was kept constant at 80 for the first iteration. The exact values for parameters c and γ — 6 and 2 were used as the initial approximations. The solution converged to 3.95 for c and - 2.44 for γ. The results are shown in Table 12A and the curve fitting in Figure 8. Three attempts were made to improve the values of the parameters.

1. Constraints were first imposed on the parameters when solving for the integration constants by simplex technique at each iteration. The constraints used were

$$4 < c(t_K) < 10$$

$$1 < \gamma(t_K) < 5$$

However, the program was terminated by the computer during the first iteration because in the Subroutine Scheck (Appendix IV, Part I) the sum of the square of the deviations of the objective functions from the mean objective function in a simplex became too large for the computer to handle.

2. Perturbation was used to stabilize the solution. The formula used was as follow

$$K(1)_n = K(0)_{n+1} + \alpha(b_S - K(0)_{n+1})$$

$$\alpha = .1$$

Table 12A. CONVERGENCE RATE OF TWO PARAMETERS, QUASILINEARIZATION WITH NOISE

ITERATIONS	$C(t_k)$	$\gamma(t_k)$
0	6.0000	2.0000
1	-1.5090	4.0426
2	-1.7664	2.7677
3	2.9674	-5.1125
4	3.3260	-2.6158
5	3.8574	-2.4569
6	3.9404	-2.4422
7	3.9586	-2.4465
8	3.9614	-2.4500
9	3.9542	-2.4474
10	3.9577	-2.4483

Time = 6.74 minutes

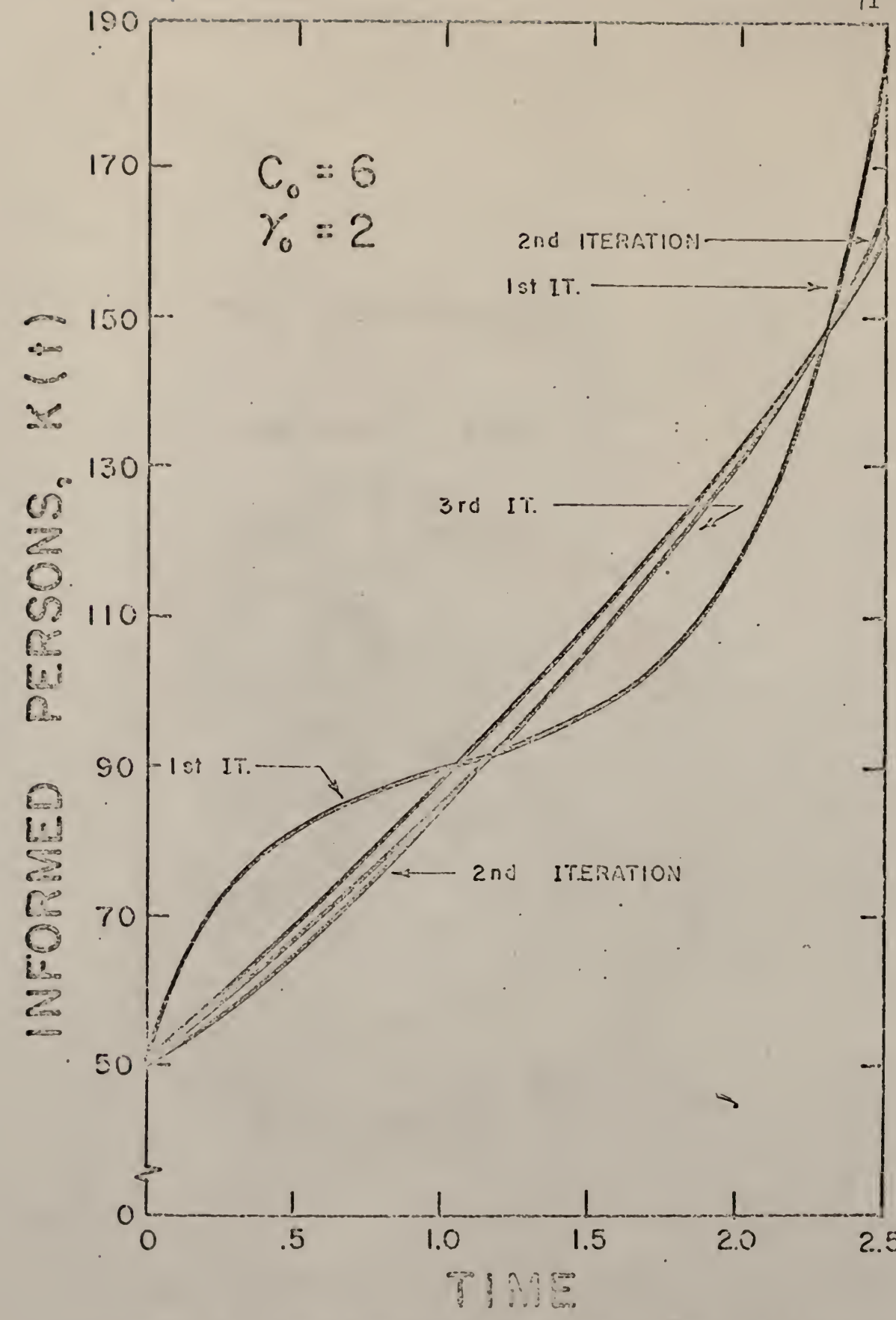

FIGURE 8. CONVERGENCE RATE FOR TWO PARAMETERS, WITH NOISE, BY QUASILINEARIZATION.

The results are shown in Table 12B. The solution seemed to converge to 3.97 for c and -2.47 for γ.

3. In order to find the effect of α, α was increased from .1 to .4. The results are given in Table 12c. It was observed that the parameters oscillated.

C-3. Numerical Integration and Pattern Search

The computational procedure was the same as that in Section B-3 under the two parameters identification except in equation (34), where $K(t)_{ED}$ used was the generated data with noise.

Numerical results

The same numerical values and initial approximations for K(t), c and γ for the data without noise were used. Two different sets of initial approximations for c and γ were used namely 1; .2 and 12;5. The solution conveyed to 6.2155; 2.0790 and 6.2183; 2.0802 respectively. In both cases the final convergence was about 3.5% off the exact parameters of 6 and 2 compared to a noise level of about 2.5%. The convergence rates for the initial approximations 1;.2 and 12;5 are shown in Table 13 and the convergence rate are shown in Figures 9. and 10 respectively.

D. Discussion

Quasilinearization did not seem to work in this particular model. From the extensive investigations in the two parameters identification the author was led to believe that in some cases Quasilinearization completely changed the response surface retaining only the same tanpent at the same point. In Table 9A the results indicated that the solution

Table 12B. CONVERGENCE RATE OF TWO PARAMETERS WITH PERTURBATION, QUASILINEARIZATION WITH NOISE

$$K(1)_n = K(0)_{n+1} + \alpha\,(b_s - K(0)_{n+1})$$

$$\alpha = .1$$

ITERATIONS	$C(t_k)$	$\gamma(t_k)$
0	6.0000	2.0000
1	-1.5090	4.0426
2	-1.7664	2.7677
3	3.0404	-5.2446
4	3.3495	-2.6488
5	3.8818	-2.4844
6	3.9664	-2.4693
7	3.9852	-2.4740
8	3.9856	-2.4762
9	3.9836	-2.4760
10	3.9795	-2.4735

Time = 6.62 minutes

Table 12C. CONVERGENCE RATE OF TWO PARAMETERS WITH PERTURBATION, QUASILINEARIZATION WITH NOISE

$$K(1)_n = K(0)_{n+1} + \alpha\ (b_s - K(0)_{n+1})$$

$$\alpha = .4$$

ITERATIONS	$C(t_k)$	$\gamma(t_k)$
0	6.0000	2.0000
1	-1.0053	2.7646
2	-0.4926	1.1872
3	1.9459	-15.0373
4	1.0414	- 0.9641
5	7.2014	- 2.2042
6	3.2252	- 1.8781
7	15.5206	- 7.9953
8	24.2528	-20.4222
9	56.8703	-53.0906
10	-15.9852	15.5956

Time = 6.49 minutes

Table 13. CONVERGENCE RATE OF TWO PARAMETERS, SEARCH AND NUMERICAL INTEGRATION WITH NOISE

EVALUATIONS	$C(t_k)$	$\gamma(t_k)$	$C(t_k)$	$\gamma(t_k)$
	1.0000	0.2000	12.0000	5.0000
10	1.7000	0.2000	12.7000	4.7000
20	1.9690	0.3485	12.7000	4.7000
30	4.2518	1.3009	11.5646	4.2237
40	6.0854	2.0246	5.8442	1.9195
50	6.1654	2.0588	6.2421	2.0925
60	6.1977	2.0718	6.1995	2.0723
70	6.2153	2.0790	6.2127	2.0779
80	6.2145	2.0786	6.2176	2.0799
90	6.2154	2.0789	6.2185	2.0803
100	6.2155	2.0790	6.2183	2.0802
110	6.2155	2.0790	6.2183	2.0802
TIME IN MINUTES	3.3		3.3	

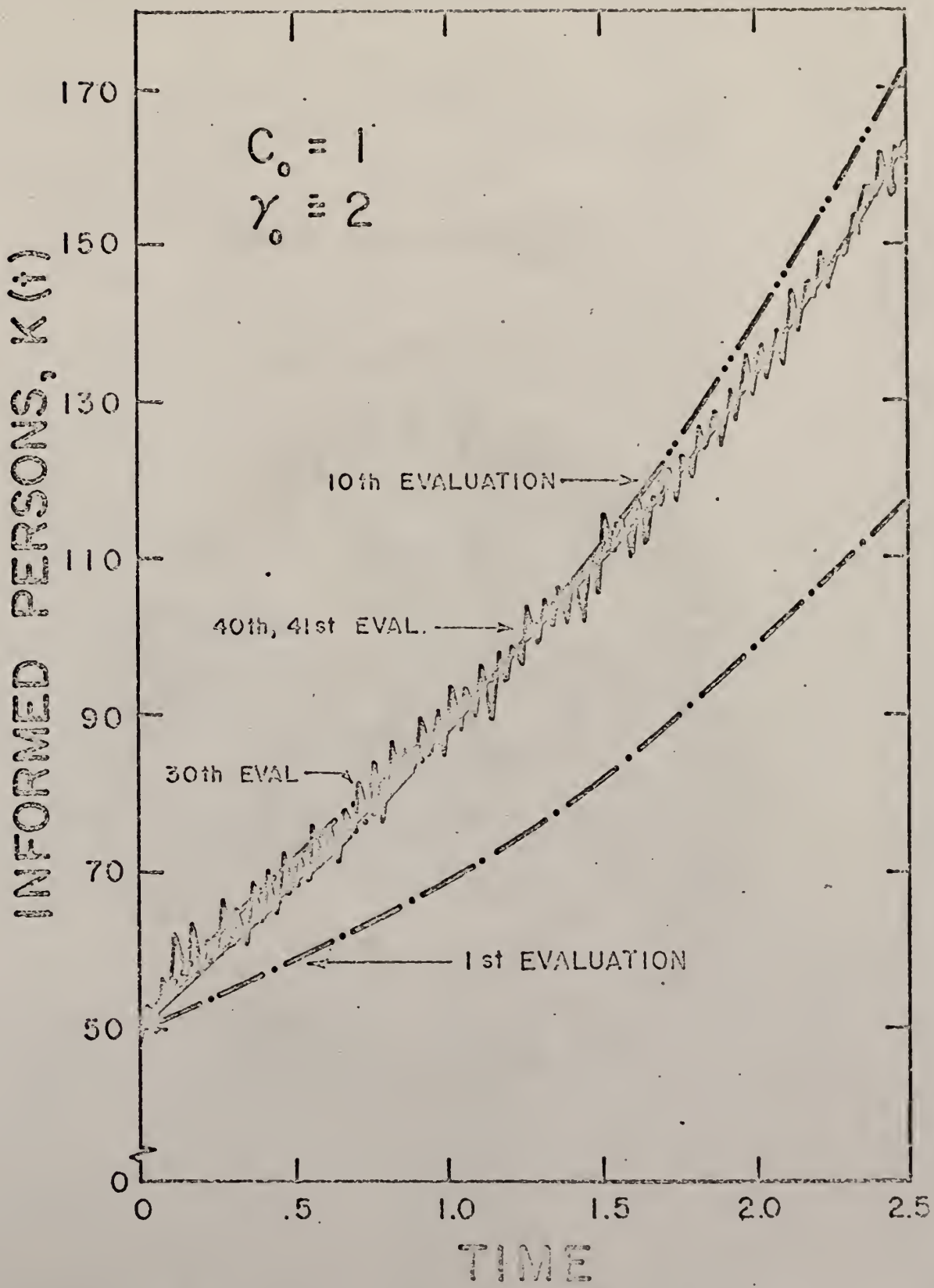

FIGURE 9. CONVERGENCE RATE FOR TWO PARAMETERS, WITH NOISE, BY SEARCH AND NUMERICAL INTEGRATION.

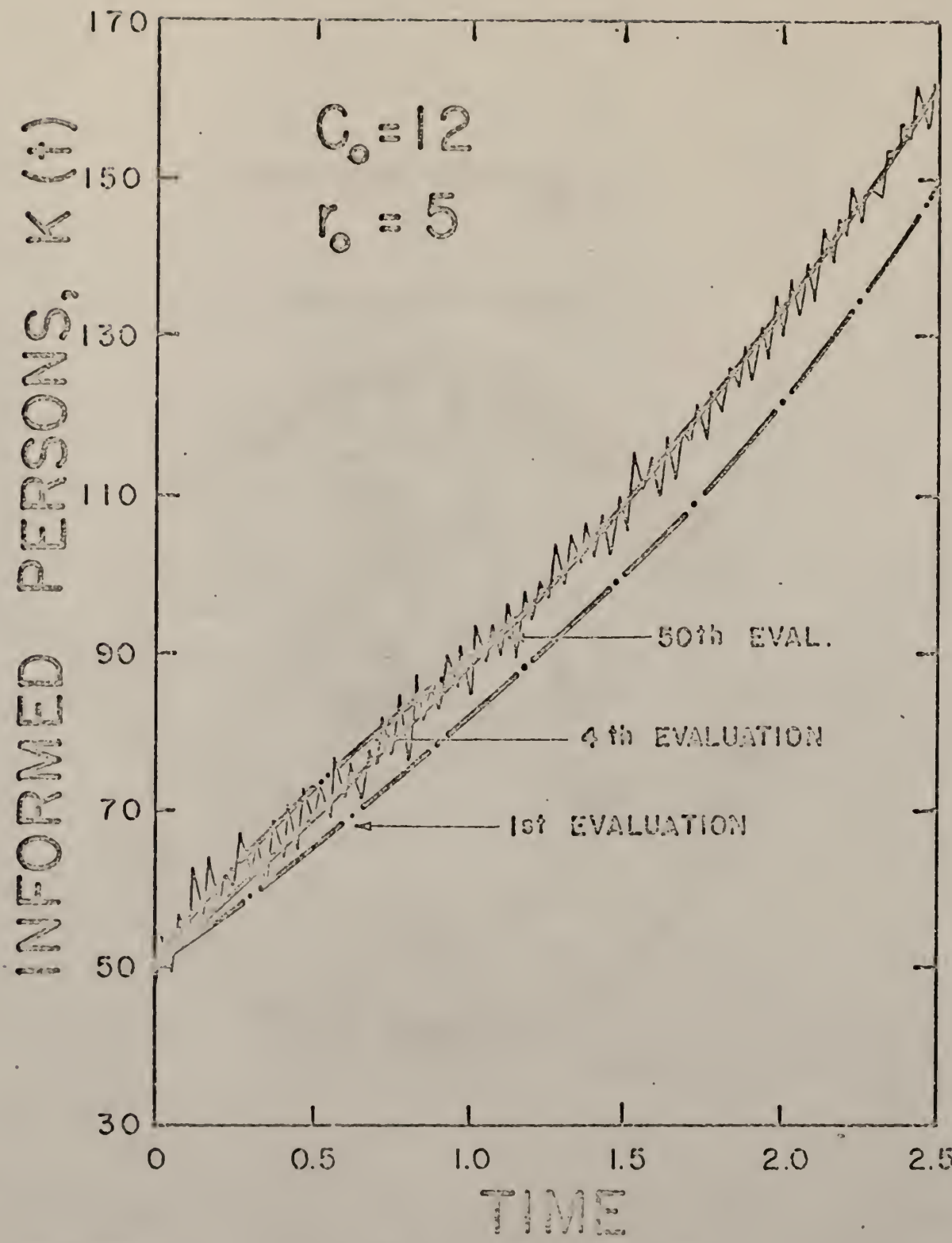

FIGURE 10. CONVEYANCE RATE FOR TWO PARAMETERS WITH NOISE BY SEARCH AND NUMERICAL INTERGRATION.

converged to a different point. The minimum point was no longer at parameters 6 and 2 nor in the vicinity between 1 and 10.5 for c and between .5 and 4 for γ as the constraints used in Table 9D where the results showed oscillation. When the data was perturbed in two different ways to obtain stability the solution converged to 4.25 and -2.76 again for parameters c and γ. This substantiated earlier prediction that a minimum did exist at this point and not at 6 and 2. This was further substantiated by the results of the two parameters with noise in the generated data where the parameters converged to 3.95 and -2.44 for c and γ, which were only slightly different from the two parameters without noise. Furthermore, the constraints used for the case with noise was more limited than that for the case without the noise. In the former case the computation was terminated before the end of the first iteration.

Numerical integration and search worked out well in this instance. However, a word of caution should be added here. The convergence depended very much on the individual model and the initial approximations of the parameters used. If there were many local minima then the choice of initial approximations was very important and vice versa. From Table 13 it was observed that the rate of convergence was very slow when approaching the minimum.

The above observations were based on the results obtained here. It might not be true in all cases. Further studies should be done if conclusive results were desired.

THREE PARAMETERS IDENTIFICATION

The growth rate, g, was also an important parameter. It indirectly affected the removal rate and the contact coefficient. Thus, it indirectly affected the means and frequency of the advertisements. Therefore, in addition to the two parameters of c and γ, a third parameter g, the growth rate was identified. The same two methods were used. Again the data used was first without noise and then contaminated with noise.

A. The Model

The model used here was the same as for two parameter identification and was reproduced below for ease of reference.

$$\frac{dK(t)}{dt} = c\,K(t)\left[1 - \frac{K(t)}{N_0 e^{gt}}\right] - \gamma K(t)$$

The same constants and step size were used.

B. Deterministic Model Without Noise

B-1. Experimental data generation.

The same data as for two parameter identification were used here and the relationship between K(t) and t was shown in Table 8.

B-2. Quasilinearization

The three constant parameters c, γ and g were identified by Quasilinearization and the least square criterion. The model was shown below.

$$\frac{dK(t)}{dt} = cK(t)\left[1 - \frac{K(t)}{N_0 e^{gt}}\right] - \gamma K(t) \qquad (35a)$$

Again the three unknown parameters c, γ and g were treated as dependent variables and as functions of the independent variable t. In addition to equation (35a) the three constant unknown parameters could be represented by the following differential equations [16]

$$\frac{dc(t)}{dt} = 0 \tag{35b}$$

$$\frac{d\gamma(t)}{dt} = 0 \tag{35c}$$

$$\frac{dg(t)}{dt} = 0 \tag{35d}$$

The initial condition for equation (35a) was

$$K(0) = 50 \tag{36}$$

The least square criterion shown below was used to determine the parameters c, γ and g so that the sum of squares of the deviations was minimized

$$Q = \sum_{s=1}^{m_1} [x(t_s) - b_s]^2 \tag{37}$$

Systems (35) and (36) were treated as a multi-point boundary-value problem.

B-2a. Computational Procedure

The parameter identification problem by Quasilinearization was composed of equations (35), (36) and (37).

The recurrence relation for the system of equations was

$$\frac{dK(t)}{dt} = c_n K_n \left(1 - \frac{K_n}{N_{0e} g_n t}\right) - \gamma_n K_n$$

$$+ (K_{n+1} - K_n) \left[c_n - \frac{2c_n K_n}{N_{0e} g_n t} - \gamma_n\right]$$

$$+ (c_{n+1} - c_n) \left[K_n - \frac{(K_n)^2}{N_{0e} g_n t}\right]$$

$$+ (\gamma_{n+1} - \gamma_n) (-K_n)$$

$$+ (g_{n+1} - g_n) \left[-\frac{c_n (K_n)^2}{N_{0e} g_n t t}\right] \qquad (38a)$$

$$\frac{d\, c_{n+1}(t)}{dt} = 0 \qquad (38b)$$

$$\frac{d\, \gamma_{n+1}(t)}{dt} = 0 \qquad (38c)$$

$$\frac{d\, g_{n+1}(t)}{dt} = 0 \qquad (38d)$$

where (n+1) was unknown functions of t and n was known functions of t obtained from the (n-1)st iterative solution.

With the superposition principle the general solutions for equations (44) were:

$$K_{n+1} = K_{p,n+1}(t) + \sum_{j=1}^{3} A_{j,n+1} K_{hj,n+1}(t) \qquad (39a)$$

$$c_{n+1}(t) = c_{p,n+1}(t) + \sum_{j=1}^{3} A_{j,n+1}\, c_{hj,n+1}(t) \tag{39b}$$

$$\gamma_{n+1}(t) = \gamma_{p,n+1}(t) + \sum_{j=1}^{3} A_{j,n+1}\, \gamma_{hj,n+1}(t) \tag{39c}$$

$$g_{n+1}(t) = g_{p,n+1}(t) + \sum_{j=1}^{3} A_{j,n+1}\, g_{hj,n+1}(t) \tag{39d}$$

Subscript p denoted particular solutions and h_1, h_2 and h_3, first, second and third set of homogeneous solutions respectively; $A_{1,n+1}$, A_{2n+1} and $A_{3,n+1}$ were integration constants

In matrix form, equation (39) became

$$K_{n+1}(t) = K_{p(n+1)}(t) + K_{h(n+1)}(t)A_{n+1} \tag{40}$$

$$K_{n+1}(t) = \begin{vmatrix} K_{n+1}(t) \\ c_{n+1}(t) \\ \gamma_{n+1}(t) \\ g_{n+1}(t) \end{vmatrix} \qquad K_{p(n+1)}(t) = \begin{vmatrix} K_{p,n+1}(t) \\ c_{p,n+1}(t) \\ \gamma_{p,n+1}(t) \\ g_{p,n+1}(t) \end{vmatrix} \tag{41}$$

$$K_{h(n+1)}(t) = \begin{vmatrix} K_{h1,n+1}(t) & K_{h2,n+1}(t) & K_{h3,n+1}(t) \\ c_{h1,n+1}(t) & c_{h2,n+1}(t) & c_{h3,n+1}(t) \\ \gamma_{h1,n+1}(t) & \gamma_{h2,n+1}(t) & \gamma_{h3,n+1}(t) \\ g_{h1,n+1}(t) & g_{h2,n+1}(t) & g_{h3,n+1}(t) \end{vmatrix} \tag{42}$$

A_{n+1} represents the integration constant vector with components $A_{1,n+1}$, $A_{2,n+1}$ and $A_{3,n+1}$.

The set of particular solutions were obtained by integrating equation (38) with the following initial values:

$$\begin{vmatrix} K_{p,n+1}(0) \\ c_{p,n+1}(0) \\ \gamma_{p,n+1}(0) \\ g_{p,n+1}(0) \end{vmatrix} = \begin{vmatrix} 50 \\ 0 \\ 0 \\ 0 \end{vmatrix} \tag{43}$$

The homogeneous forms of equation (38) were:

$$\frac{dK_{n+1}(t)}{dt} = (K_{n+1})(c_n - \frac{2c_n K_n}{N_{0e} g_n t} - \gamma_n) + (c_{n+1})(K_n - \frac{(K_n)^2}{N_{0e} g_n t}) + (\gamma_{n+1})(-K_n) + (g_{n+1})(-\frac{c_n (K_n)^2}{N_{0e} g_n t^2}) \tag{44a}$$

$$\frac{dc_{n+1}(t)}{dt} = 0 \tag{44b}$$

$$\frac{d\gamma_{n+1}(t)}{dt} = 0 \tag{44c}$$

$$\frac{dg_{n+1}(t)}{dt} = 0 \tag{44d}$$

The homogeneous solutions were obtained by integrating equation (44) with the following initial values:

$$K_{h(n+1)}(0) = \begin{vmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{vmatrix} \tag{45}$$

Equations (43) and (45) were chosen so that at t=0 Equation (39a) satisfied

Equation (36). At t=0 the following relationships were obtained

$$c_{n+1}(0) = A_{1,n+1} \tag{46a}$$

$$\gamma_{n+1}(0) = A_{2,n+1} \tag{46b}$$

$$g_{n+1}(0) = A_{3,n+1} \tag{46c}$$

Since they were constants, the relationship in Equation (46) was true for $0 \leq t \leq t_f$. Therefore,

$$c_{n+1}(t) = A_{1,n+1} \tag{47a}$$

$$\gamma_{n+1}(t) = A_{2,n+1} \tag{47b}$$

$$g_{n+1}(t) = A_{3,n+1} \tag{47c}$$

The particular and homogeneous solutions were considered known. Therefore, in the right hand side of equation (39) only the integration constants were unknown. To solve for them the least square functional was used.

$$\theta_{n+1} = \sum_{s=1}^{m_1} (K_{n+1}(t)_{cD} - K(t)_{ED})^2 \tag{48a}$$

Substituting equation (39a) into (48a)

$$\theta_{n+1} = \sum_{s=1}^{m_1} [K_{p,n+1}(t) + \sum_{j=1}^{3} A_{j,n+1} K_{hj,n+1}(t) - K(t)_{ED}]^2 \tag{48b}$$

where $K(t)_{ED}$ was the generated data which were known and shown in Table 8. The only unknown in (48b) were $A_{1,n+1}$, $A_{2,n+1}$ and $A_{3,n+1}$ which were determined by the Simplex search technique where equation (48b) became the objective function (Appendix II, Part I). Once the integration constants were known the general solution of equation (38) was obtained from equation

(39). With K_{n+1}, c_{n+1}, γ_{n+1} and g_{n+1} known an improved set of values was obtained by making n = n+1 in equation (38). The iterative procedure was continued until the solution converged to the exact parameter with a certain desired accuracy.

B-2b. Numerical Results

The numerical values used were

$$\Delta t = .025 \quad t_f = 2.5 \quad m_1 = 101$$

The first approximation of K(t) was kept constant at 80 throughout the first iteration. Exact parameters of c, γ and g, namely, 6, 2, and .4 were eimployed as the first approximations. The results are shown in Table 14A and the curve fitting in Figure 11. The solution seemed to converge to -0.98, -9.34 and 11.20 for parameters c, γ and g respectively. Constraints and perturbations were used again to improve the final values of the parameters.

1. The following constraints were used:

$$4 < c(t_K) < 10$$
$$1 < \gamma(t_K) < 5$$
$$0 < g(t_K) < 1$$

At the end of the fourth iteration parameter c and γ seemed to coverge to 4.19 and 1.00 respectively. However, the values for parameter g was still increasing. Before the end of the fifth iteration the numerical integration of the model became infinity and the computation was stopped. Results are given in Table 14B.

2. The following perturbation was used:

Table 14A. CONVERGENCE RATE OF THREE PARAMETERS, QUASILINEARIZATION WITHOUT NOISE

ITERATIONS	$C(t_k)$	$\gamma(t_k)$	$g(t_k)$
0	6.0000	2.0000	0.4000
1	-19.6564	25.4714	8.3152
2	-32.7599	26.5629	8.5849
3	- 1.8109	- 9.5871	11.1713
4	- 0.8725	- 9.4137	11.1494
5	- 0.9004	- 9.3912	11.1671
6	- 0.9274	- 9.3761	11.1769
7	- 0.9521	- 9.3622	11.1848
8	- 0.9778	- 9.3482	11.1933
9	- 0.9812	- 9.3512	11.2010
10	- 0.9935	- 9.3457	11.2056

Time = 7.25 minutes

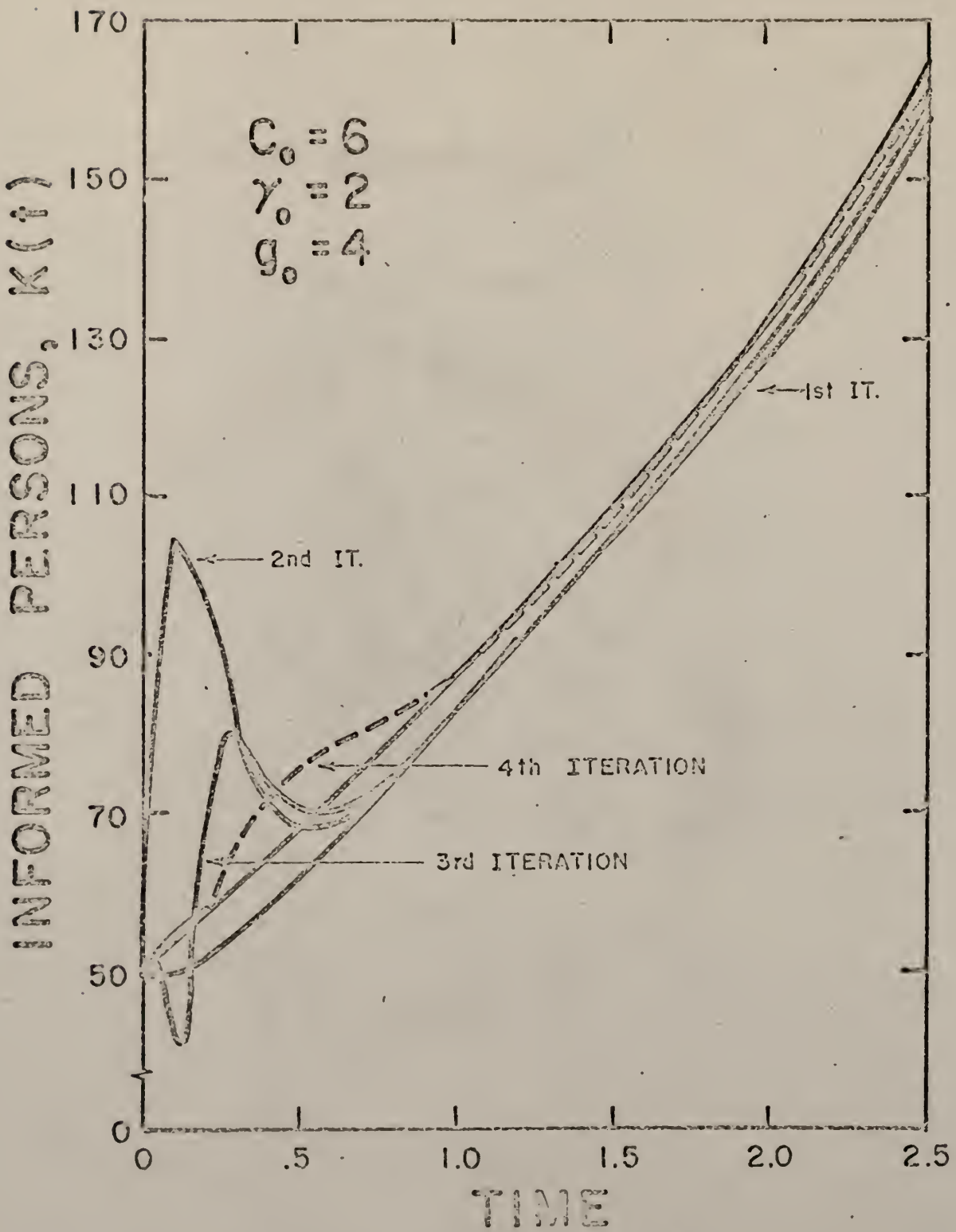

FIGURE II. CONVERGENCE RATE FOR THREE PARAMETERS BY QUASILINEARIZATION.

$$K(1)_n = K(0)_n + \alpha(K(0)_{n+1} - K(0)_n)$$

$$\alpha = .2$$

The results are shown in Table 14c. It would seem that parameters c, γ and g converged to -10.04, -5.88 and 15.11 at the end of the tenth iteration. The results of perturbation were quite different from that without perturbation.

B-3. Numerical Integration and Pattern Search

The same parameters c, γ, and g of equation (35a) were identified by numerical integration and pattern search. Equation (35a) was reproduced below

$$\frac{dK(t)}{dt} = cK(t)\left[1 - \frac{K(t)}{N_{0e}^{gt}}\right] - \gamma K(t) \tag{49}$$

with initial condition

$$K(0) = 50 \tag{50}$$

The classical least square criterion, shown below, was used again as the objective function in the search technique

$$S = Q = \sum_{S=1}^{m_1} [K_n(t)_{cD} - K(t)_{ED}]^2 \tag{51}$$

The objective was to find c, γ and g so that the sum of squares of the deviations between the solution of equation (49) and the generated data was minimized.

B-3a. Computational Procedure

The problem was composed of equation (49), (50) and (51). The

Table 14B. CONVERGENCE RATE FOR THREE PARAMETERS WITH CONSTRAINTS, QUASILINEARIZATION WITHOUT NOISE

CONSTRAINTS: $4 < C(t_k) < 10$

$1 < \gamma(t_k) < 5$

$0 < g(t_k) < 1$

ITERATIONS	$C(t_k)$	$\gamma(t_k)$	$g(t_k)$
0	6.0000	2.0000	0.4000
1	4.1999	1.0000	0.1133
2	4.1999	1.0000	0.1533
3	4.1999	1.0000	0.1933
4	4.1999	1.0000	0.2333

Time = 2.40 minutes

Table 14C. CONVERGENCE RATE OF THREE PARAMETERS WITH PERTURBATION, QUASILINEARIZATION WITHOUT NOISE

$$K(1)_n = K(0)_n + \alpha\,(K(0)_{n+1} - K(0)_n)$$

$$\alpha = .2$$

ITERATIONS	$C(t_k)$	$\gamma(t_k)$	$g(t_k)$
0	6.0000	2.0000	0.40000
1	-19.6564	25.4714	8.3152
2	-32.7600	26.5629	8.5849
3	- 6.8746	- 7.0354	13.9944
4	- 7.0285	- 7.0838	14.0290
5	- 7.0651	- 7.0601	14.0401
6	-11.2684	- 5.0684	15.3690
7	-11.7293	- 5.0951	15.3645
8	-10.0475	- 5.9762	15.0887
9	-10.0079	- 5.8898	15.1058
10	-10.0428	- 5.8838	15.1198

Time = 6.51 minutes

computational procedure was the same as for two parameters except that here it was a three dimensional search — p's had three coordinates (c, γ and g) instead of two in the case of two dimensional search (Appendix II, Part I).

B-3b. Numerical Results

The numerical values used were

$$\Delta t = .025 \quad t_f = 2.5 \quad m_1 = 101$$

Only one set of initial approximations for c, γ and g were used namely 11, 4 and .6. It was chosen arbitrarily. It was found that the solution converged to the exact parameters of 6, 2 and 4. The convergence rate of the constant parameters is shown in Table 15 and the convergence rate is shown in Figure 12.

C. Deterministic Model with Noise.

The same parameters c, γ and g of equation (35a) were identified. However, noise was imposed on the data. The same two methods were used.

C-1. Experimental data generation

The same data with noise for two parameters identification were used here and they are shown in Table 11.

C-2. Quasilinearization computational procedure was the same as in section B-2 of three parameters identification except that in equation (48b), $K(t)_{ED}$ used was the generated data with noise.

Numerical Results

The numerical values used were the same as without noise. The results are given in Table 16A and the curve fitting in Figure 13. The integration

Table 15. CONVERGENCE RATE OF THREE PARAMETERS, SEARCH AND NUMERICAL INTEGRATION WITHOUT NOISE

EVALUATIONS	$C(t_k)$	$\gamma(t_k)$	$g(t_k)$
	11.0000	4.0000	0.6000
10	11.0000	6.0000	0.6000
20	12.2431	5.0206	0.4705
30	13.0117	4.4395	0.3626
40	12.4279	4.8615	0.4277
50	12.5076	4.8056	0.4121
60	12.5198	4.7707	0.4108
70	12.5051	4.7792	0.4127
80	12.4898	4.7760	0.4126
90	12.4582	4.7557	0.4122
100	12.2043	4.6587	0.4127
110	10.8767	4.1097	0.4127
120	7.1399	2.5183	0.4095
130	7.7101	2.7531	0.4090
140	7.2238	2.5201	0.4030
150	6.3461	2.1519	0.4019
160	6.0320	2.0129	0.4002
170	5.9307	1.9701	0.3996
180	6.0219	2.0095	0.4001
190	6.0098	2.0043	0.4000
200	5.9963	1.9984	0.4000
205	6.000	1.9999	0.3999

TIME IN MINUTES: 6.90

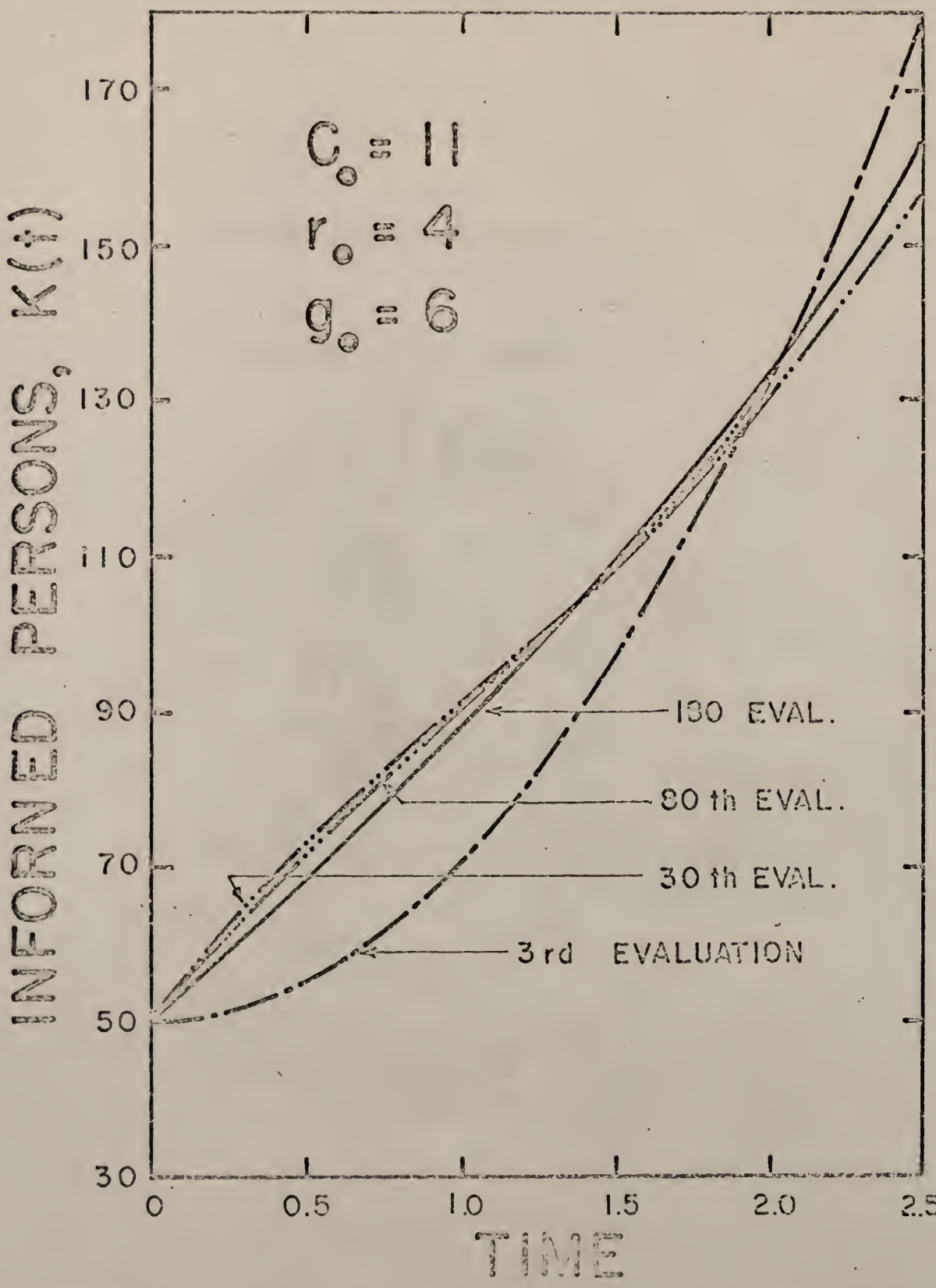

FIGURE 12. CONVERGENCE RATE FOR THREE PARAMETERS, BY SEARCH AND NUMERICAL INTEGRATION.

constants oscillated and the computation was terminated after the sixth iteration, because the numerical integration of the model became infinity in the seventh iteration. Constraints and perturbation were used again to improve the solution.

1. The following constraints were used:

$$4 < c(t_K) < 10$$

$$1 < \gamma(t_K) < 5$$

$$0 < g(t_K) < 1$$

Parameters c and γ seemed to converge to 4.1999 and 1.0000 respectively at the end of the fourth iteration but the value for parameter g was still increasing. However, in the fifth iteration the numerical integration of the model became infinity and the computation was terminated. Results are given in Table 16B.

2. The perturbation used was as below

$$K(1)_n = K(0)_n + \alpha(K(0)_{n+1} - K(0)_n)$$

$$\alpha = .5$$

The results are shown in Table 16c. At the end of ten iterations the solution seemed to be more stable than before but the results still did not give much of a sign of convergence.

C-3. Numerical Integration and Pattern Search

Computational Procedure

The computational procedure was the same as in section B-3 of three parameters identification except in equation (51), $K(t)_{ED}$ used was the generated data with noise.

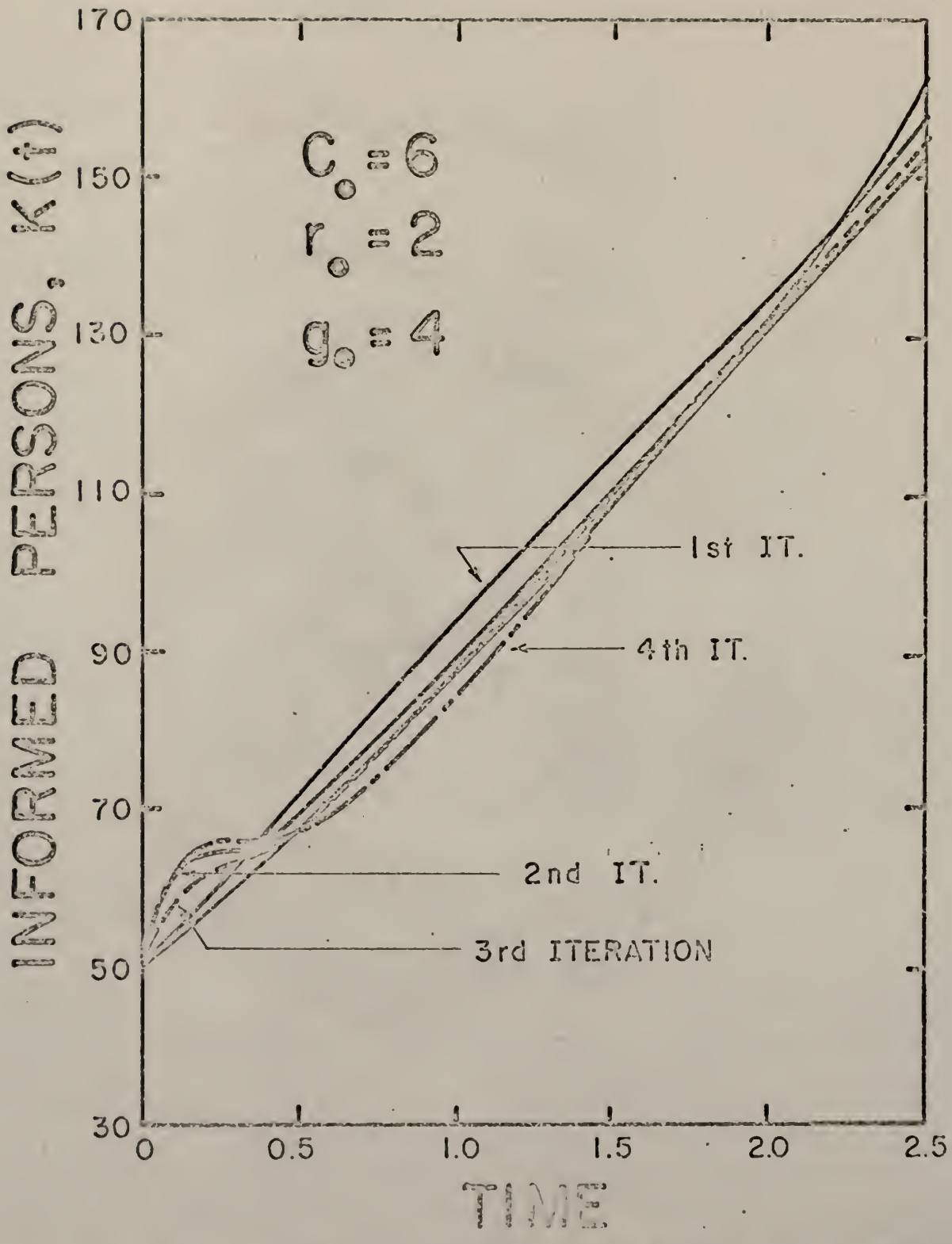

FIGURE 15. CONVERGENCE RATE FOR THREE PARAMETERS, WITH NOISE, BY QUASILINEARIZATION.

Table 16A. CONVERGENCE RATE OF THREE PARAMETERS, QUASILINEARIZATION WITH NOISE

ITERATIONS	$C(t_k)$	$\gamma(t_k)$	$g(t_k)$
0	6.0000	2.0000	0.4000
1	0.8652	-1.2595	0.0279
2	2.3725	-1.5420	0.6657
3	0.7351	-0.9984	0.7127
4	3.4211	-1.5696	0.7296
5	0.2537	-0.7641	0.6517
6	2.7040	0.7291	-3.6554

TIME IN MINUTES: 5.63

Table 16B. CONVERGENCE RATE OF THREE PARAMETERS WITH CONSTRAINTS, QUASILINEARIZATION WITH NOISE

CONSTRAINTS: $4 < C(t_k) < 10$

$1 < \gamma(t_k) < 5$

$0 < g(t_k) < 1$

ITERATIONS	$C(t_k)$	$\gamma(t_k)$	$g(t_k)$
0	6.0000	2.0000	0.4000
1	4.1999	1.0000	0.1133
2	4.1999	1.0000	0.1533
3	4.1999	1.0000	0.1933
4	4.1999	1.0000	0.2333

TIME IN MINUTES = 2.46

Table 16C. CONVERGENCE RATE OF THREE PARAMETERS WITH PERTURBATION, QUASILINEARIZATION WITH NOISE

$$K(1)_n = K(0)_n + \alpha\ (K(0)_{n+1} - K(0)_n)$$

$$\alpha = .5$$

ITERATIONS	$C(t_k)$	$\gamma(t_k)$	$g(t_k)$
0	6.0000	2.0000	0.4000
1	0.8652	-1.2595	0.0279
2	2.3725	-1.5420	0.6657
3	1.7071	-1.4902	0.7039
4	1.7582	-1.4579	0.7207
5	1.7187	-1.4408	0.7387
6	1.6804	-1.4225	0.7592
7	1.6421	-1.4040	0.7808
8	1.6052	-1.3859	0.8032
9	2.1420	-1.5719	0.7289
10	1.0768	-1.1953	0.7567

TIME IN MINUTES = 6.57

Numerical Results.

The same numerical values and the initial approximations for K(t), c, γ and g for the data without noise were used. Only one set of initial approximations was used namely, 11, 4, .6. The solution converged to 12,4851, 4.8090 and 0.4145. It was found that when $c(t_K)$ shot to 13.0117 at the 30th evaluation (Table 13) the solution converged to another minimum point. Constraints were then imposed on c as follows

$$1 < c < 12$$

The solution now converged to 6.4877, 2.2326 and 0.4045. However, it took 70 more evaluations (approximately 2 minutes) to converge. The rates of convergence with and without constraints are shown in Table 17 and the convergence rate with constraint is shown in Figure 14.

D. Discussion

Conclusion cannot be drawn here from Quasilinearization than that for the two parameters case. The results shown in Table 16A, B and C did not even indicate any sign of convergence. It was very unstable due to the complexity of the problem.

In the numerical integration and search the effect of local minimum was seen here in the case with noise. When c went over 12, the solution converged to a different point namely, 12.4851, 4.8090 and 0.4145. However, when constraint was imposed in c (between 1 and 12) the solution converged to 6.4877, 2.2326 and 0.4045 slightly perturbed from that of without noise.

Table 17. CONVERGENCE RATE OF THREE PARAMETERS SEARCH AND NUMERICAL INTEGRATION WITH NOISE

WITH CONSTRAINT $1 < C(t_k) < 12$				WITHOUT CONSTRAINT		
EVALUATIONS	$C(t_k)$	$\gamma(t_k)$	$g(t_k)$	$C(t_k)$	$\gamma(t_k)$	$g(t_k)$
	11.0000	6.0000	0.6000	11.0000	6.0000	0.6000
10	11.0000	6.0000	0.6000	11.0000	6.0000	0.6000
20	11.2979	3.8481	0.3930	12.2431	5.0206	0.4705
30	10.9437	4.3643	0.4293	13.0117	4.4395	0.3626
40	11.0414	4.2199	0.4187	12.4279	4.8615	0.4277
50	11.0240	4.1670	0.4121	12.4993	4.8006	0.4105
60	11.0350	4.1810	0.4129	12.5011	4.7904	0.4122
70	11.0361	4.1870	0.4130	12.4920	4.8030	0.4140
80	11.0335	4.1836	0.4130	12.4875	4.8070	0.4142
90	11.0308	4.1840	0.4131	12.4863	4.8082	0.4143
100	11.0121	4.1746	0.4129	12.4858	4.8086	0.4144
110	10.8549	4.1017	0.4124	12.4850	4.8091	0.4145
120	10.1745	3.7956	0.4105	12.4851	4.8090	0.4145
130	9.0874	3.3225	0.4078	12.4851	4.8090	0.4145
140	7.0253	2.4500	0.4038			
150	6.4330	2.2025	0.4032			
160	6.1423	2.0817	0.4028			
170	6.3272	2.1596	0.4033			
180	6.4813	2.2295	0.4045			
190	6.4870	2.2318	0.4044			
200	6.4877	2.2326	0.4045			
TIME IN MINUTES		7.03			4.55	

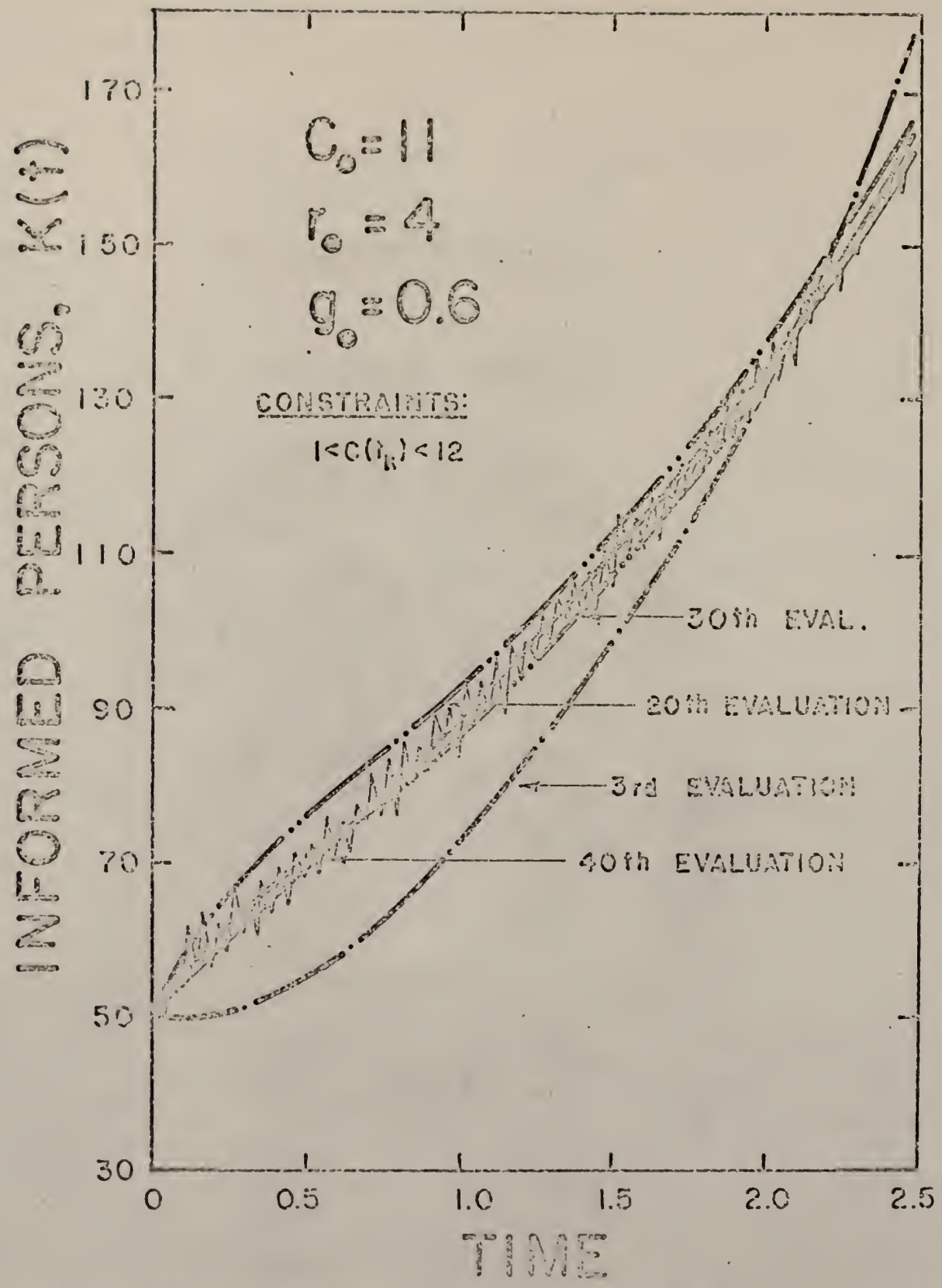

FIGURE 14. CONVERGENCE RATE FOR THREE PARAMETERS WITH NOISE BY SEARCH AND NUMERICAL INTERGRATION.

TABLE 18 SUMMARY OF THE RESULTS OF QUASILINEARIZATION

No. of Parameters	Noise	Exact Parameter	Initial Approximations	Constraints and/or Pert.	Number of Iterations	Final Value of Parameter	IBM 360/50 Time in Mins.
One (c)	None	2	6	None	6	1.9982	1.16
			10	None	6	1.9982	1.16
			20	None	6	1.9982	1.16
	3.44%	Approx. 2	6	None	7	1.9783	1.21
			10	None	7	1.9783	1.21
			20	None	7	1.9783	1.21
Two(c,v)	None	6,2	6,2	None	10 terminated	4.23;-2.73	5.10
	None	6,2	6,2	Constraints	at 4	Oscillation	3.01
	None	6,2	6,2	α = .2	10	4.25;-2.76	5.65
	None	6,2	6,2	α = .05	20	4.24;-2.74	9.09
	None	6,2	6,2	Constraint α = .1	10	Oscillation	5.45
	None	6,2	6,2	α = .1	10	Oscillation	6.35
	None	6,2	6,2	α = .4	18	4.23;-2.73	10.16
	2.55%	App. 6,2	6,2	None	10	3.95;-2.44	6.74
				α = .1	10	3.97;-2.47	6.62
				α = .4	10	Oscillation	6.49
Three (c,v,g)	None	6,2,.4	6,2,.4	None	10	-0.99 9.34 11.20	7.25
				Constraint	terminated at 4	4.1999 1.0000 0.2333	2.40
				α = .2	10	-10.04 - 5.88 15.11	6.51
	2.55%	Approx. 6,2,.4	6,2,.4	None	6	Oscillation	5.63
				Constraint	4	4.1999 1.0000 0.2333	2.46
				α = .5	10	OSC.	6.57

TABLE 19 SUMMARY OF THE RESULTS OF SEARCH AND NUMERICAL INTEGRATION

No of Parameters	Noise	Exact Parameter	Initial Approximations	Number of Evaluations	Final Value of Parameters		IBM 360/50 Time
One (c)	None	2	6	10	2.0000		.556
	None	2	10	20	2.0000		.835
	None	2	20	20	2.0000		.835
	3.44%	Approx. 2	6	10	2.0000		.598
			10	20	2.0000		.798
			20	20	2.0000		.798
Two(c,v)	None	6.2	1;.2	100	5.9999	1.9999	3.5000
			12; 5	100	5.9999	1.9999	3.5000
	2.55%	Approx. 6,2	1;.2	110	6.2155	2.0790	3.3000
			12; 5	110	6.2183	2.0802	3.3000
Three (c,v,g)	None	6,2,.4	11,4,.6	205	6.0000;1.9999;0.3999		6.9000
	2.55%	Approx. 6,2,.4	11,4,.6	200	12.4851;4.8090;0.4145		4.5500
		(with constraint 1<C<12)			6.4877;2.2326;0.4045		7.0300

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Appendix I

Quasilinearization

Given a nonlinear first order differential equation [15, 17]

$$\frac{dx}{dt} = g(x,t), \tag{1}$$

with boundary condition

$$x(0) = \alpha \tag{2}$$

Function g(x,t) is nonlinear. Equation (1) could be solved by Runge-Kutta-Gill method since it is a first order ordinary differential equation.

The function, g(x,t), could be linearized around x = y as follows,

$$g(x,t) = g(y,t) + (x-y)\left| \frac{\partial g(x,t)}{\partial x} \right|_{x=y} \tag{3}$$

which is the Taylor Series with second and higher order terms omitted. x and y are functions of independent variable t. Equation (1) and (3) are combined.

$$\frac{dx}{dt} = g(y,t) + (x-y)g_y(y,t) \tag{4}$$

where $g_y(y,t)$ represents the partial differentiation of the function g(y,t) with respect to y and is equal to

$$\left| \frac{\partial g(x,t)}{\partial x} \right|_{x=y}$$

y is considered as a known function of t and x as the unknown and so equation (4) is a linear differential equation with variable coefficients. The boundary condition for equation (4) is given by equation (2).

A recurrence relation could now be constructed. An initial approximation for $y(t)$ is chosen which is named $x_0(t)$. The first approximation for $y(t)$ is substituted into equation (4) and this first order linear differential equation with boundary condition of $x(0) = \alpha$ is solved for $x(t)$ by the step by step integration of Rung-Kutta-Gill method. This newly determined function is called $x_1(t)$. $x_1(t)$. $x_1(t)$ is then used as $y(t)$ in equation (4) and an improved $x(t)$ is obtained. This new improved function is called $x_2(t)$, which is substituted into equation (4) for $y(t)$ and an improved $x_3(t)$ is obtained. The procedure is continued until the desired accuracy is obtained. The recurrence relation could be written as

$$\frac{dx_1(t)}{dt} = g(x_0(t),t) + (x_1(t) - x_0(t))\, g_{x_0}(x_0(t),t), \tag{5}$$

$$\frac{dx_2(t)}{dt} = g(x_1(t),t) + (x_2(t) - x_1(t))\, g_{x_1}(x_1(t),t), \tag{6}$$

$$\frac{dx_N(t)}{dt} = g(x_{N-1}(t),t) + (x_N(t) - x_{N-1}(t))\, g_{x_{N-1}}(x_{N-1}(t),t). \tag{7}$$

The boundary condition given by equation (2) is used in equation (5) through (7).

This convergence rate of the quasilinearization technique is quadratic in the sense that each iteration approximately doubles the number of digits of accuracy.

Now the following set of n simultaneous first-order nonlinear ordinary differential equations is considered [15, 17]

$$\frac{dx_i}{dt} = g_i(x_1, x_2, \ldots, x_n, t), \qquad i = 1, 2, \ldots, n \tag{9}$$

with appropriate boundary conditions. The vector form of equation (9) could be linearized around point $\underline{y} = (y_1, y_2, y_3, \ldots, y_n)$ as follows

$$\frac{d\underline{x}}{dt} = \underline{g}(\underline{y}, t) + \underline{J}(\underline{y})(\underline{x}-\underline{y}), \tag{10}$$

where $\underline{x}$, and $\underline{g}$ are in vector form and represent the vectors $(x_1, x_2, \ldots, x_n)$ and $(g_1, g_2, \ldots, g_n)$ respectively. The Jacobi matrix, $\underline{J}(\underline{y})$, is defined by

$$\underline{J}(\underline{y}) = \begin{vmatrix} \frac{\partial g_1}{\partial y_1} & \frac{\partial g_1}{\partial y_2} & \cdots & \frac{\partial g_1}{\partial y_n} \\ \frac{\partial g_2}{\partial y_1} & \frac{\partial g_2}{\partial y_2} & \cdots & \frac{\partial g_2}{\partial y_n} \\ \vdots & \vdots & & \vdots \\ \frac{\partial g_n}{\partial y_1} & \frac{\partial g_n}{\partial y_2} & \cdots & \frac{\partial g_n}{\partial y_n} \end{vmatrix}$$

in which $\frac{\partial g_i}{\partial y_i}$ represent the partial differentiation of $g_i(y_1, y_2, \ldots, y_{n,t})$ with respect to y_j. In matrix form, equation (10) could be written as

$$\begin{vmatrix} \frac{dx_2}{dt} \\ \vdots \\ \frac{dx_n}{dt} \end{vmatrix} = \begin{vmatrix} g_2(y_1,y_2,\ldots,y_{n,t}) \\ \vdots \\ g_n(y_1,y_2,\ldots,y_{n,t}) \end{vmatrix} + \begin{vmatrix} (x_1-y_1)\frac{\partial g_2}{\partial y_1} + (x_2-y_2)\frac{\partial g_2}{\partial y_2} + \ldots + (x_n-y_n)\frac{\partial g_2}{\partial y_n} \\ \vdots \\ (x_1-y_1)\frac{\partial g_n}{\partial y_1} + (x_2-y_2)\frac{\partial g_n}{\partial y_n} + \ldots + (x_n-y_n)\frac{\partial g_n}{\partial y_n} \end{vmatrix} \tag{11}$$

The recurrence relation for the system of equations, equation (11), in general, could be written in the same form as equation (5) through (7).

$$\begin{aligned} \frac{dx_{i,N}}{dt} &= g_i(x_{1,N-1}, x_{2,N-1}, \cdots, x_{n,N-1,t}) \\ &+ (x_{1,N} - x_{1,N-1}) \frac{\partial g_1}{\partial x_{1,N-1}} + \ldots \\ &+ (x_{n,N} - x_{n,N-1}) \frac{\partial g_1}{\partial x_{n,N-1}}, \quad i = 1, 2, \ldots, n, \\ &\qquad\qquad\qquad\qquad\qquad\qquad N = 0, 1, 2, \ldots \end{aligned} \tag{12}$$

Here the first subscript, i, denotes the subscript of the dependent variables $x_1, x_2, \ldots, x_n$, and the second subscript, N, denotes the Nth iteration. In equation (12) $x_{i,N}$ is considered as an unknown function and $x_{i,N-1}$ as a known function of t obtained from the (N-1)st iterative solution. Thus, equation (10) or (12) would always be linear.

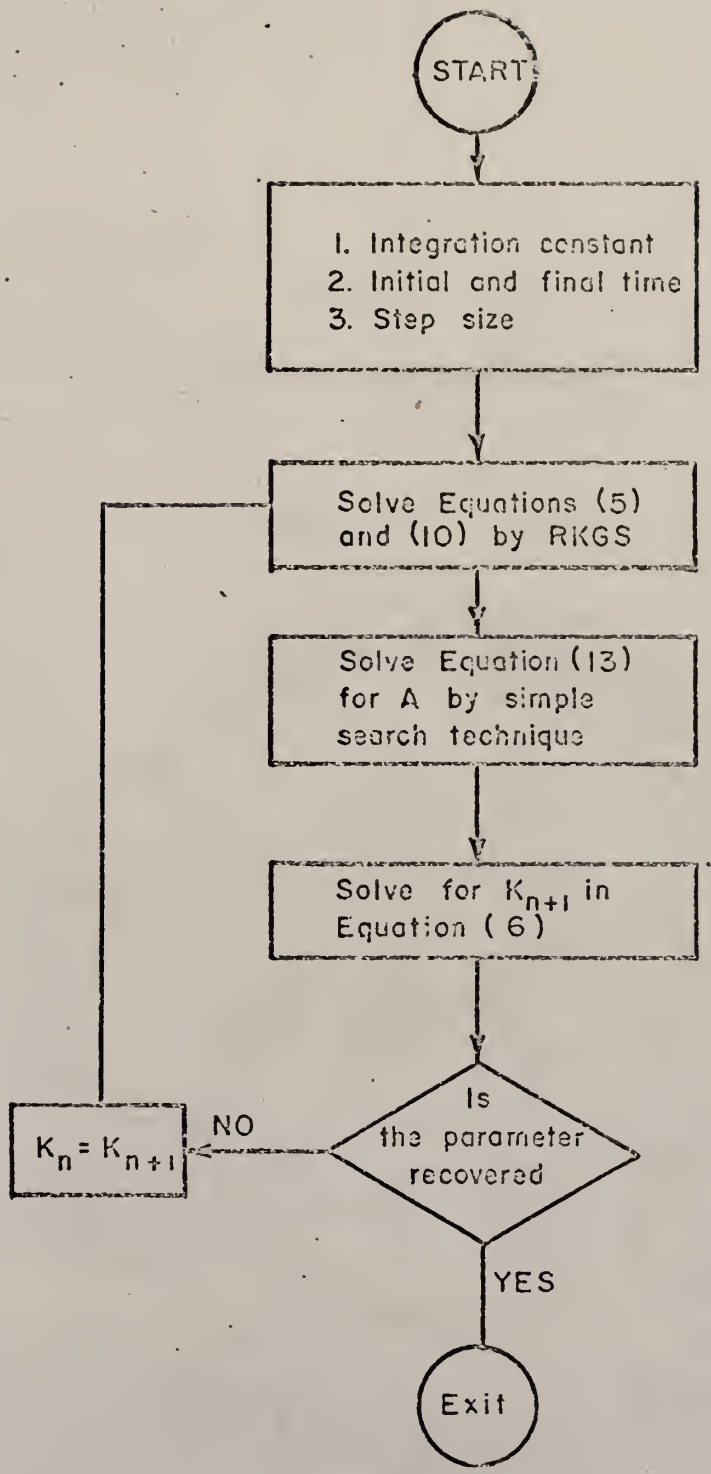

FIGURE 15. COMPUTER FLOW CHART OF QUASILINEARIZATION METHOD

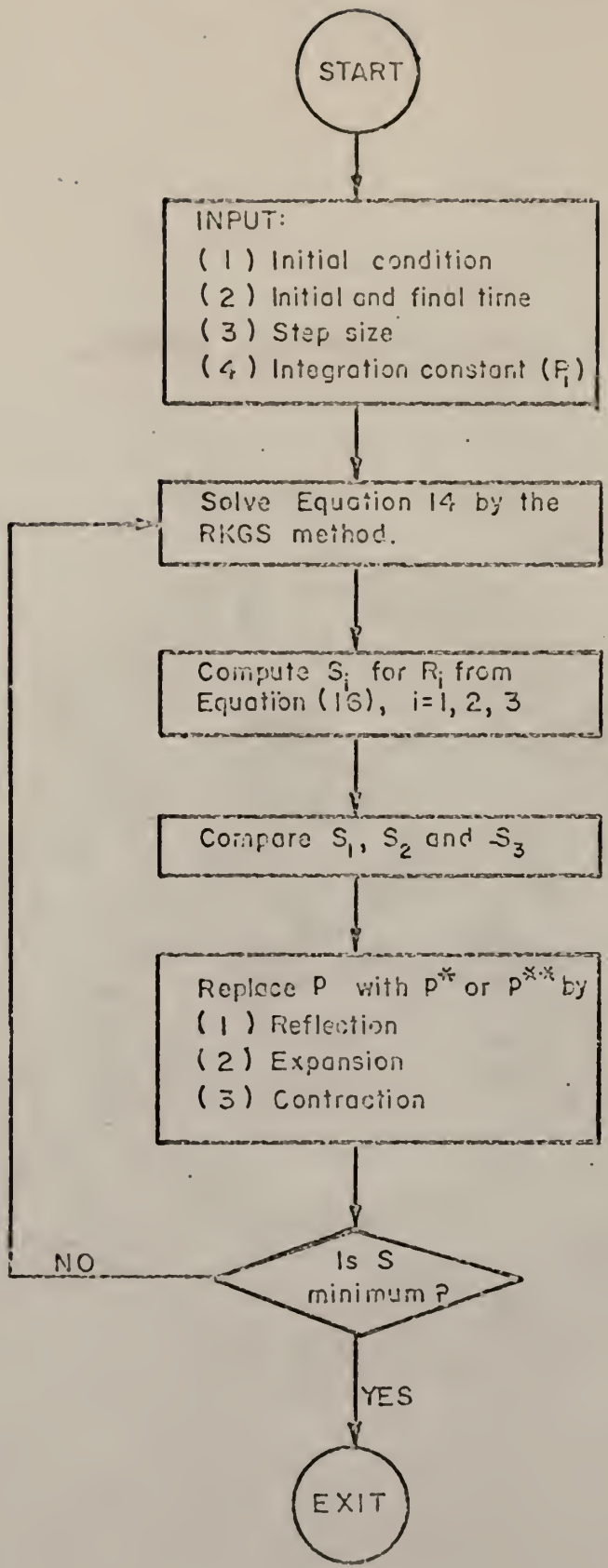

FIGURE 16. COMPUTER FLOW CHART FOR NUMERICAL ITERATION AND SEARCH.

Appendix II

Simplex Search Technique

The Simplex search technique used in this work was developed by Nelder and Mead [20]. This method depends on the comparison of function values at the (n+1) vertices of a general simplex, followed by the replacement of the vertex with the highest value by another point.

The following notations were used

P_n = n^{th} point in n-dimensional space defining the current "simplex"

S_n = the function value at P_n

h = suffix such that S_h was maximum value of S (h for "high")

ℓ = suffix such that S_ℓ = minimum value of S (ℓ for "low")

$\bar{P}$ = centroid of the points with $i \neq h$

P_iP_j = distance between P_i to P_j

A two dimensional problem is used to illustrate this method. Minimize objective function = S = $f_1(x,y)$

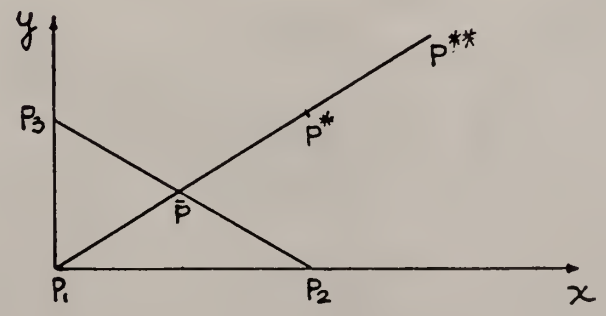

Figure 17. Simplex search technique diagram

Step I Starting with any three arbitrary points to form a simplex: P_1, P_2 and P_3. Their respective objective function are evaluated as S_1, S_2 and S_3 and compared. It is supposed that S values in the decending order are $S_1 = S_h$, S_2, $S_3 = S_\ell$. The minimum value of the objective function is along the line $P_1\bar{P}$ and opposite $P_1 (P_1 = P_h)$.

Step II The new point to replace P_h is along $P_h\bar{P}$ and in the opposite end of P_h. This new point is obtained by reflection and denoted by P^*.

$$P^* = (1 + \alpha)\bar{P} - \alpha P_h \tag{1}$$

where α is a positive constant, the reflection coefficient and

$$P^*\bar{P} = \alpha P_h\bar{P} \tag{2}$$

If S^* lied between S_h and S_ℓ then P_h was replaced by P^* and the search was started again with the new simplex.

Step III If $S^* < S_\ell$, that is if reflection has produced a new minimum then P^* is expanded to P^{**} by the relation

$$P^{**} = \gamma P^* + (1-\gamma)\bar{P} \tag{3}$$

the expansion coefficient

$$\gamma = \frac{P^{**}\bar{P}}{P^*\bar{P}} \tag{4}$$

and is greater than unity.

If $S^{**} < S_\ell$, P_h is replaced by P^{**} and Step I is repeated. But if $S^{**} > S_\ell$, the expansion fails and P^{**} is discarded. P_h is

then replaced by P^* only and Step I is repeated.

Step IV If on reflecting P_h to P^* it is found that $S^* > S_\ell$ for all $i \neq h$, i.e. that replacing P_h by P^* leaves S^* the maximum. A new P_h is defined which could be either the old P_h or P^*, whichever has the lower S value and forms

$$P^{**} = \beta P_h + (1-\beta)\bar{P} \ . \tag{5}$$

The contraction coefficient β lies between 0 and 1 and

$$\beta = \frac{P^{**}\bar{P}}{P\bar{P}} \tag{6}$$

P^{**} then replaces P_h and Step I is restarted. If $S^{**} > \min(S_h; S^*)$, i.e. the contracted point is worse than the worse of P_h and P^*, it is a failed contraction. In this case all P_i's are placed by $(P_i + P_\ell)/2$ and the process is restarted.

A failed expansion could be taken as overshooting the valley so that P^{**} is well upon the opposite side. A failed contraction occurs when the valley is curved and one point of the simplex is much farther from the valley bottom than the others. Contraction might then cause the reflected point to move away from the valley bottom instead of towards it. Further contractions would be useless. These actions contract the simplex towards the lowest point and would eventually bring all the points into the valley. α,β and γ determines the volume of simplex to be changed.

The criterion chosen to stop the process is to compare the "standard error" of the objective function in the form

$\sqrt{\{\sum(S_i - \bar{S})^2/n\}}$ with a desired value. If it falls below the desired value the process is stopped.

If there are constraints on the parameters then any parameter violating the constraint is given a large objective function value and contraction is then followed to bring the parameter inside the constraints.

Nelder and Mead found that the best values for α,β and γ were 1, 1/2 and 2.

A computer flow chart of Simplex search technique is shown in Figure 18.

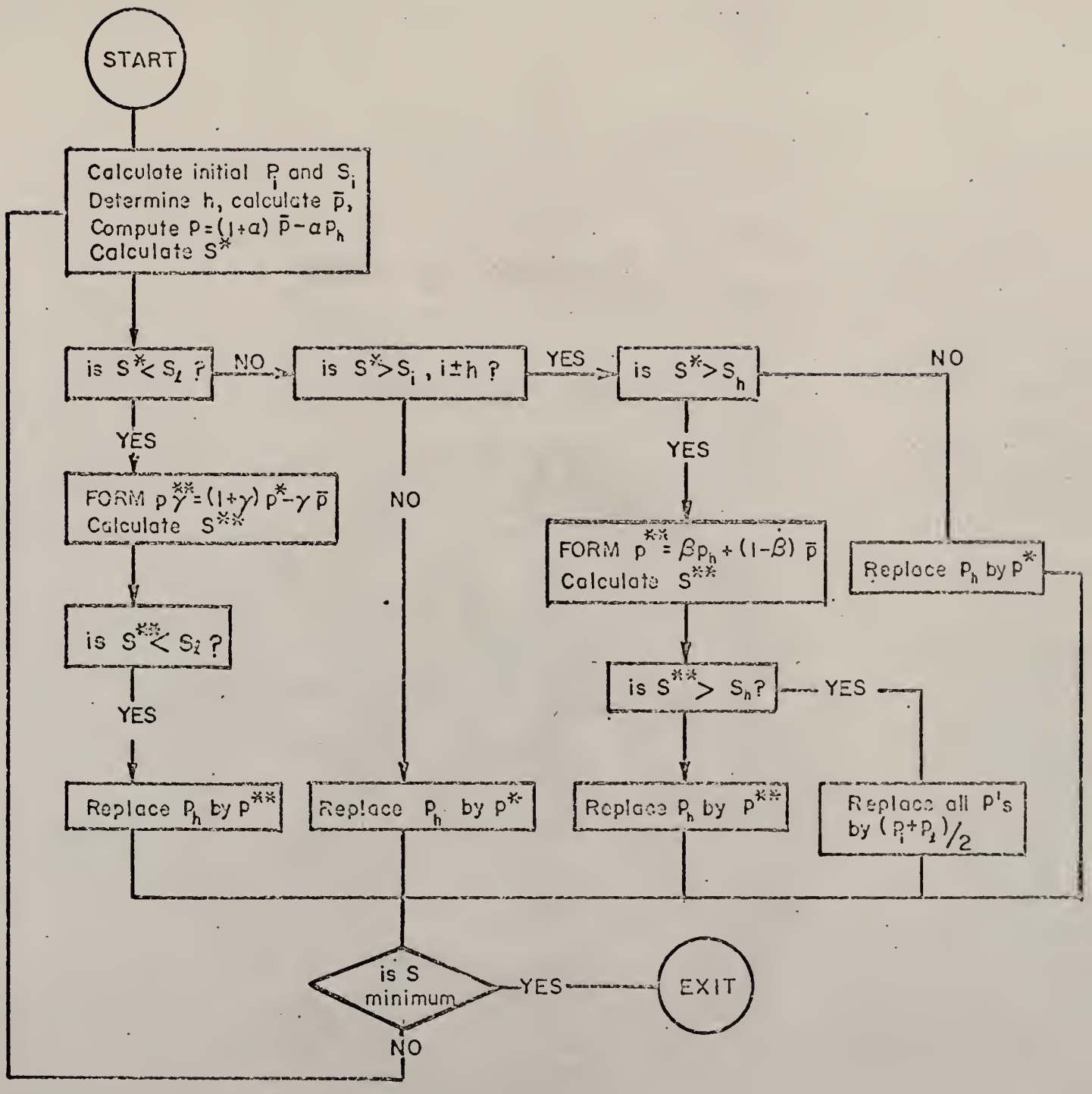

FIGURE 18. COMPUTER FLOW CHART OF SIMPLEX SEARCH TECHNIQUE.

Appendix III

Runge-Kutta-Gill Method (RKGS)

In solving the differential equations in this work the IBM subroutine, Runge-Kutta-Gill numerical integration method (RKGS) was used [12, 21].

The purpose of the Runge-Kutta-Gill method is to obtain an approximate solution of a system of first order ordinary differential equations with given initial values. It is a fourth-order integration procedure which is stable and self-starting — only the functional values at a previous point are required to obtain the functional values ahead. For this reason it is easy to change the step size h at any step in the calculations. Control of accuracy and adjustment of the step size h is done by comparing the results due to double and single step size 2h and h.

Given the system of first-order ordinary differential equations:

$$y_1' = \frac{dy_1}{dx} = f_1(x, y_1, y_2, \ldots, y_n)$$

$$y_2' = \frac{dy_2}{dx} = f_2(x, y_1, y_2, \ldots, y_n)$$

$$y_n' = \frac{dy_n}{dx} = f_n(x, y_1, y_2, \ldots, y_n)$$

and the initial values:

$$y_1(x_0) = y_{1,0},\ y_2(x_0) = y_{2,0},\ \ldots,\ y_n(x_0) = y_{n,0}$$

and using the following vector notations:

$$y(x) = \begin{vmatrix} y_1(x) \\ y_2(x) \\ \vdots \\ y_n(x) \end{vmatrix}, \quad F(x,y) = \begin{vmatrix} f_1(x,y) \\ f_2(x,y) \\ \vdots \\ f_n(x,y) \end{vmatrix}, \quad y_0 = \begin{vmatrix} y_{1,0} \\ y_{2,0} \\ \vdots \\ y_{n,0} \end{vmatrix}$$

where y, F and y_0 are column vectors, the given problem appears as follow:

$$y' = \frac{dy}{dx} = F(x,y), \quad y(x_0) = y_0$$

Thus, starting at x_0 with $y(x_0) = y_0$ and vector $Q_0 = 0$, the resulting vector $y_4 = y(x_0+h)$ is computed by the following formulae:

$$K_1 = h \cdot F(x_0,y_0); \; y_1 = y_0 + \frac{1}{2}(K_1 - 2Q_0);$$

$$Q_1 = Q_0 + 3\left|\frac{1}{2}(K_1 - 2Q_0)\right| - \frac{1}{2}K_1$$

$$K_2 = h \cdot F(x_0 + \frac{h}{2}, y_1); \; y_2 = y_1 + (1 - \overline{\frac{1}{2}})(K_2 - Q_1);$$

$$Q_2 = Q_1 + 3\left|(1 - \overline{\frac{1}{2}})(K_2 - Q_1)\right| - (1 - \overline{\frac{1}{2}})K_2$$

$$K_3 = h \cdot F(x_0 + \frac{h}{2}, y_2); \; y_3 = y_2 + (1 + \overline{\frac{1}{2}})(K_3 - Q_2);$$

$$Q_3 = Q_2 + 3\left|(1 + \overline{\frac{1}{2}})(K_3 - Q_2)\right| - (1 + \overline{\frac{1}{2}})K_3$$

$$K_4 = h \cdot F(x_0 + h,\ y_3);\quad y_4 = y_3 + \frac{1}{6}(K_4 - 2A_3);$$

$$Q_4 = Q_3 + 3\left|\frac{1}{6}(K_4 - 2Q_3)\right| - \frac{1}{2}K_4$$

where K_1, K_2, K_3, K_4, y_1, y_2, y_3, y_4, Q_1, Q_2, Q_3, Q_4 are all column vectors with n components. If the procedure is carried out with infinite precision (no rounding errors), vector Q_4 defined above would be zero. In practice this is not true, and Q_4 represents approximately three times the round off error in y_4 accumulated during one step. To compensate for this accumulated roundoff, Q_4 is used as Q_0 for the next step. Also $(x_0 + h)$ and y_4 serve as x_0 and y_0 respectively at the next step.

For initial control of accuracy, an approximation for $y(x_0 + 2h)$ called $y^{(2)}(x_0 + 2h)$ was computed using the step size 2h, and then an approximation called $y^{(1)}(x_0 + 2h)$, using two times the step size h. From these two approximations, a test value δ for accuracy is generated in the following way:

$$\delta = \frac{1}{15}\sum_{i=1}^{n} a_i \cdot \left|y_i^{(1)} - y_i^{(2)}\right|$$

where the coefficients a_i are error weights specified in the input of the procedure.

Test value δ is an approximate measure for the local truncation error at point $x_0 + 2h$. If δ is greater than a given tolerance ε_2, increment h is halved and the procedure starts again at the point x_0. If δ is less than ε_2, the results $y^{(1)}(x_0 + h)$ and $y^{(1)}(x_0 + 2h)$ are assumed to be correct. They are then handed, together with $x_0 + h$ and $x_0 + 2h$ and the derivatives at these points — the values of $F\left|x_0 + h,\ y^{(1)}(x_0 + h)\right|$

and $F\left|x_0 + 2h,\ y^{(1)}(x_0 + 2h)\right|$ respectivel — to a user-supplied output subroutine.

If δ is less than $\varepsilon_1 = \varepsilon_2/50$, the next step is carried out with the doubled increment. However, care is taken in the procedure that the increment never becomes greater than the increment h specified as an input parameter, and further that all points $x_0 + j \cdot h$(where $j = 1, 2, \ldots$) which are situated between the lower and upper bound of the integration interval are included in the output. Finally, the increment of the last step of the procedure is chosen in such a way that the upper bound of the integration interval is reached exactly.

This control of accuracy was applied only in the generation of the experimental data for one and two parameters. The experimental data for three parameters were the same as for two parameters. This control of accuracy was not used when solving the differential equations both in the Quasilinearization and Simplex pattern search technique methods.

Summary of the Computational Procedure of RKGS

a. Input

1. Lower and upper bound of the initial increment of the independent variable, upper bound ε_2 of the local truncation error.
2. Initial values of the dependent variables and weights for the local truncation errors in each component of the dependent variables.
3. The number of differential equations in the system.
4. As external subroutine subprograms, the computation of the right-hand side of the system of differential equations; for flexibility in output, an output subroutine.
5. An auxiliary storage array named AUX with 8 rows and n columns.

b. Order of the calculation

1. j is set equal to 1
2. i is set equal to 0.
3. y'_{ij} is computed

$$y'_{ij} = K_{ij} = hf_i(y_{0,j-1}, y_{1,j-1}, \cdots, y_{n,j-1})$$

$$= hf_{i,j-1}$$

4. Step (3) is repeated for i = 1, 2, ..., n
5. i is set to 0 again
6. y_{ij} and q_{ij} are computed.

$$y_{ij} = y_{i,j-1} + a_j(K_{ij} - b_j Q_{i,j-1})$$

$$Q_{ij} = Q_{i,j-1} + 3[a_j(K_{ij} - b_j Q_{i,j-1})] - c_j K_{ij}$$

where

$$a_1 = 1/2 \qquad b_1 = 2 \qquad c_1 = 1/2$$

$$a_2 = 1 - \sqrt{1/2} \qquad b_2 = 1 \qquad c_2 = 1 - \sqrt{1/2}$$

$$a_3 = 1 + \sqrt{1/2} \qquad b_3 = 1 \qquad c_3 = 1 + \sqrt{1/2}$$

$$a_4 = 1/6 \qquad b_4 = 2 \qquad c_4 = 1/2$$

Initially, $Q_{i0}(x_0) = 0$ for all i; therefore, in advancing the solution,

$$Q_{i0}(x_t) = Q_{i4}(x_{t-1}) \qquad t = 1, 2, \ldots$$

To eliminate bias, Q_{i1} and Q_{i4} should be rounded in opposite directions, one rounded up and the other rounded down. Of fundamental importance in controlling the growth of round-off errors is that K_{ij} and Q_{ij} be obtained to the same order of accuracy, with errors of the order of h times the error in y_{ij}.

7. Step (6) is repeated for i = 1, 2, ..., n.

8. Steps (2) - (7) is repeated for j = 2, 3 and 4.

c. Output

$$y_{i4} = \bar{y}_i(x_0 + h)$$

To advance the solution, step (1) - (8) are repeated, letting the current y_{i4} be the initial values y_{i0} for the next step.

A computer flow chart for Runge-Kutta-Gill method is shown on Figure 19.

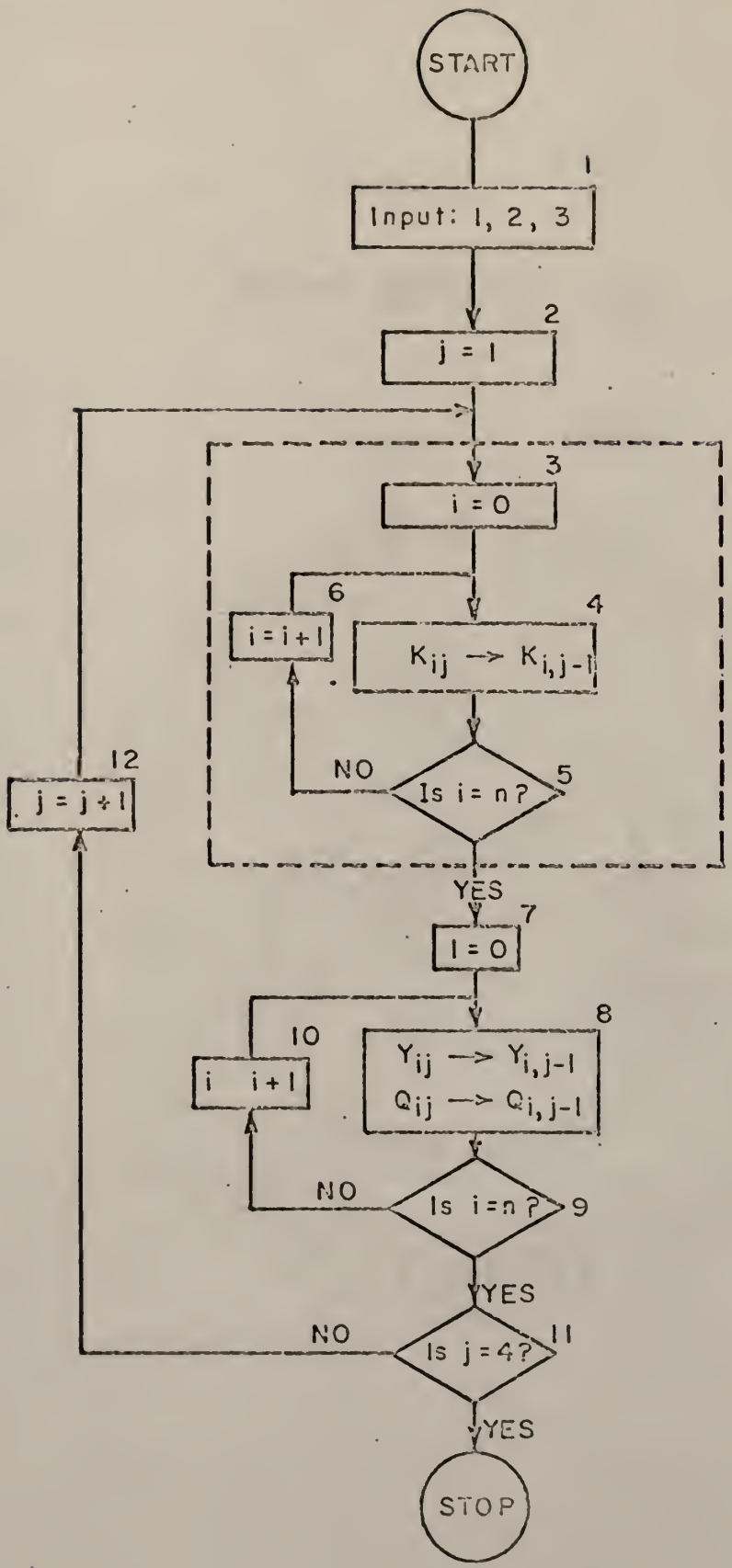

FIGURE 19. COMPUTER FLOW FOR RUNGE-KUTTA-GILL METHOD.

APPENDIX IV. COMPUTER PROGRAM FOR THREE PARAMETERS WITHOUT NOISE BY QUASILINEARIZATION

```
      EXTERNAL FCT,OUTP,ORDER,CNTROD,SCHECK,SUBNAM,RANDU
      DIMENSION PRMT(3),Y(4),DERY(4),AUX(6,4)
      DIMENSION BS(102),PART(102),HOMO1(102),HOMO2(102),HOMO3(102)
      DIMENSION PHOY1(5),PHOY2(5),PHOY3(5),PHOY4(5)
      DIMENSION AP(102),W(505)
      DIMENSION DLTVX(27,28),S(30),DCVX(27,30)
      COMMON AA,AK,BK,IX,MM,L,N,W,AP,PART,HOMO1,BS,HOMO2,HOMO3
    1 FORMAT(//,40X,11H ITERATION ,I3)
    2 FORMAT(/,19X,5H TIME,18X,15H SUBJECT MATTER)
    3 FORMAT(16X,F12.6,14X,E18.9,8X,E18.9)
    4 FORMAT(F16.8)
    5 FORMAT(4E16.8)
    6 FORMAT(4F16.8)
    7 FORMAT(/,27X,5H PART,16X,6H HOMO1,17X,6H HOMO2)
  101 FORMAT(10I5)
  102 FORMAT(9E8.4)
  103 FORMAT(/16H EVALUATION NO =I5/)
  104 FORMAT(6E13.6)
  105 FORMAT(20X,E18.9,5X,E18.9,5X,E18.9)
  106 FORMAT(/,29X,2HKA,20X,3H KB,21X,3H KB)
      READ(1,6) (PRMT(I),I=1,3)
      READ(1,6) EQUNO,VARIA
      READ(1,6) CC,CP,CQ
      READ(1,6) (PHOY1(M),M=1,4)
      READ(1,6) (PHOY2(M),M=1,4)
      READ(1,6) (PHOY3(M),M=1,4)
      READ(1,6) (PHOY4(M),M=1,4)
      READ(1,101)NDIM,NOPT,NDIMP1,MAXNO,METHOD
      READ(1,102)ERROR,SUPLIM
      READ(1,102)((DLTVX(I,J),I=1,NDIM),J=1,NDIMP1)
      READ(1,4) (BS(I),I=1,101)
      READ(1,104) (DCVX(I,1),I=1,NDIM)
      IY=1
      AA=6.0
      AK=2.0
      BK=0.40
    8 JJ=1
      IX=1
      WRITE(3,106)
      WRITE(3,105) AA,AK
   11 WRITE(3,1) JJ
      M=1
      MM=1
      N=1
      NDIM=EQUNO
   12 L=1
      Y(1)=PHOY1(M)
      Y(2)=PHOY2(M)
      Y(3)=PHOY3(M)
      IF(NDIM-2) 16,16,15
```

```
   15 Y(4)=PRCY4(M)
   16 CALL RKGS(PRMT,Y,DERY,FCT,OUTP,NDIM,AUX)
      MM=MM+1
      M=M+1
      IF(M-EQUNC) 12,12,17
   17 IF(IX-10) 28,28,45
   28 IX=IX+1
      N=1
      DO 29 I=1,101
      PART(I)=W(N)
      N=N+1
   29 CONTINUE
      N=102
      DO 30 I=1,101
      HOMO1(I)=W(N)
      N=N+1
   30 CONTINUE
      N=203
      DO 31 I=1,101
      HOMO2(I)=W(N)
      N=N+1
   31 CONTINUE
      IF(NDIM-2) 33,33,32
   32 N=304
      DO 107 I=1,101
      HOMO3(I)=W(N)
      N=N+1
  107 CONTINUE
   33 NDIM=VARIA
      WRITE(3,101)NDIM,NOPT,NDIMP1,MAXNO,METHOD
      WRITE(3,104)ERROR,SUPLIM
      WRITE(3,104)(DCVX(I,1),I=1,NDIM)
      WRITE(3,104)((DLTVX(I,J),I=1,NDIM),J=1,NDIMP1)
      CALL RKCHEN(NDIM,METHOD,MAXNO,ERROR,SUPLIM,DLTVX,DCVX,S,KK)
      WRITE(3,104)S(NDIM+2),(DCVX(I,NDIM+2),I=1,NDIM)
      WRITE(3,104)((DCVX(I,J),I=1,NDIM),J=1,NOPT)
      WRITE(3,104)(S(I),I=1,NOPT)
      WRITE(3,103)KK
      AA=DCVX(1,NDIM+2)
      AK=DCVX(2,NDIM+2)
      IF(NDIM-2) 35,35,111
  111 BK=DCVX(3,NDIM+2)
   35 XX=0.0
      WRITE(3,2)
      IF(NDIM-2) 36,36,38
   36 DO 37 I=1,101
      AP(I)=PART(I)+AA*HOMO1(I)+AK*HOMO2(I)
      WRITE(3,3) XX,AP(I)
      XX=XX+PRMT(3)
   37 CONTINUE
      GO TO 40
   38 DO 39 I=1,101
      AP(I)=PART(I)+AA*HOMO1(I)+AK*HOMO2(I)+BK*HOMO3(I)
      WRITE(3,3) XX,AP(I)
      XX=XX+PRMT(3)
   39 CONTINUE
   40 WRITE(3,106)
```

```
      AA=CC*AA
      AK=CP*AK
      IF(NDIM-2) 42,42,41
   41 BK=CO*BK
      WRITE(3,105) AA,AK,BK
      GO TO 44
   42 WRITE(3,105) AA,AK
   44 JJ=JJ+1
      GO TO 11
   45 IY=IY+1
      IF(IY-3) 46,46,43
   46 DCVX(1,1)=.65
      GO TO 8
   43 STOP
      END
```

```
      SUBROUTINE RKGS(PRMT,Y,DERY,FCT,OUTP,NDIM,AUX)
      DIMENSION Y(1),DERY(1),A(4),B(4),C(4),PRMT(1),AUX(6,1)
      DIMENSION AP(102),W(505)
      COMMON AA,AK,BK,IX,MM,L,N,W,AP,PART,HOMO1,BS,HOMO2,HOMO3
      X=PRMT(1)
      XEND=PRMT(2)
      H=PRMT(3)
      A(1)=.5
      A(2)=.2928932
      A(3)=1.707107
      A(4)=.1666667
      B(1)=2.
      B(2)=1.
      B(3)=1.
      B(4)=2.
      C(1)=.5
      C(2)=.2928932
      C(3)=1.707107
      C(4)=.5
      DO 3 I=1,NDIM
      AUX(3,I)=0.
    3 AUX(6,I)=0.0
      CALL FCT(X,Y,DERY)
      CALL OUTP(X,Y,DERY)
    9 J=1
   10 AJ=A(J)
      BJ=B(J)
      CJ=C(J)
      DO 11 I=1,NDIM
      R1=H*DERY(I)
      R2=AJ*(R1-BJ*AUX(6,I))
      Y(I)=Y(I)+R2
      R2=R2+R2+R2
   11 AUX(6,I)=AUX(6,I)+R2-CJ*R1
      IF(J-4) 12,15,15
   12 J=J+1
      IF(J-3) 13,14,13
   13 X=X+.5*H
   14 CALL FCT(X,Y,DERY)
      GO TO 10
   15 DO 17 I=1,NDIM
   17 AUX(6,I)=AUX(3,I)
      CALL OUTP(X,Y,DERY)
      IF(X-XEND) 9,16,16
   16 RETURN
      END
```

```
      SUBROUTINE FCT(X,Y,DERY)
      DIMENSION PRMT(1),Y(1),DERY(1)
      DIMENSION AP(102),W(505)
      COMMON AA,AK,BK,IX,MM,L,N,W,AP,PART,HOMO1,BS,HOMO2,HOMO3
      IF(MM-1) 1,1,2
    1 E=1.0
      GO TO 3
    2 E=0.0
    3 ANO=100.
      EXPTM=EXP(-BK*X)
      TERM1=((AA*AP(L))*(1.-(AP(L)/(ANO*EXP(BK*X))))-AK*AP(L))*E
      TERM2=(Y(1)-E*AP(L))*(AA-((2.*AA*AP(L))/(ANO*EXP(BK*X))))-AK
      TERM4=(Y(3)-AK)*(-AP(L))
      TERM3=(Y(2)-E*AA)*(AP(L)-(AP(L)*AP(L)/(ANO*EXP(BK*X))))
      TERM5=(Y(4)-BK)*((-AA*AP(L)*AP(L))*(-X)*EXPTM/ANO)
      DERY(1)=TERM1+TERM2+TERM3+TERM4+TERM5
      DERY(2)=0.0
      DERY(3)=0.0
      DERY(4)=0.0
      RETURN
      END
```

```
      SUBROUTINE OUTP(X,Y,DERY)
      DIMENSION PRMT(1),Y(1),DERY(1)
      DIMENSION AP(102),W(505)
      COMMON AA,AK,BK,IX,MM,L,N,W,AP,PART,HOMO1,BS,HOMO2,HOMO3
      IF(IX-1) 701,701,701
  701 W(N)=Y(1)
      N=N+1
      IF(X-.0249) 704,702,702
  702 L=L+1
  704 RETURN
      END
```

```
      SUBROUTINE GKCHEN(NDIM,METHOD,MAXNO,ERROR,SUPLIM,DLTVX,DCVX,S,KK)
      DIMENSION DLTVX(27,28),C(28),DCVX(27,30),S(30),CNTROX(27)
      DIMENSION AP(102),W(505)
      COMMON AA,AK,BK,IX,MM,L,N,W,AP,PART,HOMO1,BS,HOMO2,HOMO3
  110 FORMAT(/19H THIS IS NEW METHOD/)
  111 FORMAT(/16H THIS IS SIMPLEX/)
  112 FORMAT(/12H THIS IS BOX/)
  113 FORMAT(/16H ****WARNING****/)
  114 FORMAT(  50H INADEQUATE GIVEN MAX. NO FOR FUNCTION EVALUATION,)
  115 FORMAT(47H INCREASING THE MAXNO OR CHANGING THE STEP SIZE/)
      GO TO (116,117,118),METHOD
  116 JMCHEN=1
      KCHEN=1
      ALPHO=1.0
      BETA=0.5
      COEFF=1.2
      GAMMA=2.0
      WRITE(3,110)
      GO TO 1
  117 JMCHEN=1
      KCHEN=2
      ALPHO=1.0
      BETA=0.5
      GAMMA=2.0
      WRITE(3,111)
      GO TO 1
  118 JMCHEN=NDIM
      ALPHO=1.3
      BETA=0.5
      WRITE(3,112)
    1 J=1
      KK=1
      CALL SUBNAM(NDIM,J,SUPLIM,S,DCVX,KK)
      K=NDIM+JMCHEN
      KLT1=K-1
      DO 3  J=2,K
      DO 2 I=1,NDIM
    2 DCVX(I,J)=DCVX(I,1)+DLTVX(I,J-1)
      CALL SUBNAM(NDIM,J,SUPLIM,S,DCVX,KK)
    3 CONTINUE
    4 M=K
      ALPHA=ALPHO
      CALL ORDER(M,NDIM,S,DCVX)
      DO 5  I=1,KLT1
    5 C(I)=1.
      CALL CNTROD(NDIM,KLT1,C,CNTROX,DCVX)
    6 DO 7  I=1,NDIM
    7 DCVX(I,K+1)=CNTROX(I)+ALPHA*(CNTROX(I)-DCVX(I,K))
      J=K+1
      CALL SUBNAM(NDIM,J,SUPLIM,S,DCVX,KK)
      IF(KK-MAXNO)8,8,36
    8 GO TO (9,9,23),METHOD
    9 IF(S(K+1)-S(1))10,10,23
   10 DO 11 I=1,NDIM
   11 DCVX(I,K+2)=CNTROX(I)+GAMMA*(DCVX(I,K+1)-CNTROX(I))
      J=K+2
```

```
      CALL SUBNAM(NDIM,J,SUPLIM,S,DCVX,KK)
      IF(KK-MAXNO)12,12,36
   12 GO TO (16,13),KCHEN
   13 IF(S(K+2)-S(1))14,14,21
   14 S(K)=S(K+2)
      DO 15 L=1,NDIM
   15 DCVX(L,K)=DCVX(L,K+2)
      GO TO 35
   16 IF(S(K+2)-S(K+1))17,17,21
   17 S(K)=S(K+2)
      DO 18 L=1,NDIM
   18 DCVX(L,K)=DCVX(L,K+2)
      M=K
      CALL ORDER(M,NDIM,S,DCVX)
      CALL SCHECK(K,SUM,NDIM,S)
      IF(SUM-ERROR)37,37,19
   19 CVALUE=2*NDIM-1
      DO 20 I=1,KLT1
      C(I)=CVALUE
   20 CVALUE=2*NDIM-2
      CALL CNTROD(NDIM,KLT1,C,CNTROX,DCVX)
      ALPHA=ALPHO*COEFF
      GO TO 6
   21 S(K)=S(K+1)
      DO 22 L=1,NDIM
   22 DCVX(L,K)=DCVX(L,K+1)
      GO TO 35
   23 IF(S(K+1)-S(K-1))21,21,24
   24 IF(S(K+1)-S(K))25,25,27
   25 S(K)=S(K+1)
      DO 26 I=1,NDIM
   26 DCVX(I,K)=DCVX(I,K+1)
   27 DO 28 I=1,NDIM
   28 DCVX(I,K+1)=CNTROX(I)+BETA*(DCVX(I,K)-CNTROX(I))
      J=K+1
      CALL SUBNAM(NDIM,J,SUPLIM,S,DCVX,KK)
      IF(KK-MAXNO)29,29,36
   29 IF(S(K+1)-S(K))30,30,32
   30 S(K)=S(K+1)
      DO 31 I=1,NDIM
   31 DCVX(I,K)=DCVX(I,K+1)
      GO TO 35
   32 DO 34 J=2,K
      DO 33 I=1,NDIM
   33 DCVX(I,J)=(DCVX(I,1)+DCVX(I,J))/2.
      CALL SUBNAM(NDIM,J,SUPLIM,S,DCVX,KK)
   34 CONTINUE
      IF(KK-MAXNO)35,35,36
   35 CALL SCHECK(K,SUM,NDIM,S)
      IF(SUM-ERROR)37,37,4
   36 WRITE(3,113)
      WRITE(3,114)
      WRITE(3,115)
      GO TO 40
   37 DO 38 I=1,KLT1
   38 C(I)=1.
      CALL CNTROD(NDIM,KLT1,C,CNTROX,DCVX)
      DO 39 I=1,NDIM
   39 DCVX(I,K+1)=CNTROX(I)
```

```
      J=K+1
      CALL SUBNAM(NDIM,J,SUPLIM,S,DCVX,KK)
   40 RETURN
      END
```

```
      SUBROUTINE SUBNAM(NDIM,J,SUPLIM,S,DCVX,KK)
      DIMENSION S(30),DCVX(27,30),X(27),XOPT(27),HOMO2(102)
      DIMENSION AP(102),W(505),PART(102),HOMO1(102),BS(102),HOMO3(102)
      COMMON AA,AK,BK,IX,MM,L,N,W,AP,PART,HOMO1,BS,HOMO2,HOMO3
    1 FORMAT(31H THE OPTIMUM FUNCTION VALUE IS E13.6)
    2 FORMAT(6E13.6)
    3 FORMAT(10I4)
      IF(J-1)4,4,5
    4 KCONT=10
      ERR=10.
      GO TO 6
    5 KK=KK+1
    6 DO 7  I=1,NDIM
      X(I)=DCVX(I,J)
    7 CONTINUE
      T1=0.0
      DO 20 I=1,101
      T2=X(1)*HOMO1(I)
      T3=X(2)*HOMO2(I)
      T4=X(3)*HOMO3(I)
   20 T1=T1+(PART(I)+T2+T3+T4-BS(I))**2
      T=T1
      S(J)=T
      IF(J-1) 9,9,11
    9 DO 10 I=1,NDIM
      XOPT(I)=X(I)
   10 CONTINUE
      SOPT=T
      IF(J-1)17,17,12
   11 IF(S(1)-S(J))12,9,9
   12 IF(KK-KCONT)14,13,13
   13 WRITE(3,1)SOPT
      WRITE(3,2)(XOPT(I),I=1,NDIM)
      WRITE(3,3)KK
      KCONT=KCONT+10
   14 IF(S(J)-ERR)15,15,17
   15 WRITE(3,1)SOPT
      WRITE(3,2)(XOPT(I),I=1,NDIM)
      WRITE(3,3)KK
      ERR=ERR*0.1
      GO TO 17
   16 S(J)=SUPLIM
   17 RETURN
      END
```

```
      SUBROUTINE ORDER(M,NDIM,S,DCVX)
      DIMENSION S(30),DCVX(27,30)
      DIMENSION AP(102),W(505)
      COMMON AA,AK,BK,IX,MM,L,N,W,AP,PART,HOMO1,BS,HOMO2,HOMO3
      K=M
      KLT1=K-1
      DO  5 I=1,KLT1
      M=M-1
      DO  4 J=1,M
      IF(S(M+1)-S(J))2,2,4
    2 A=S(M+1)
      S(M+1)=S(J)
      S(J)=A
      DO  3 L=1,NDIM
      B=DCVX(L,M+1)
      DCVX(L,M+1)=DCVX(L,J)
      DCVX(L,J)=B
    3 CONTINUE
    4 CONTINUE
    5 CONTINUE
      RETURN
      END
```

```
      SUBROUTINE CNTROD(NDIM,KLT1,C,CNTROX,DCVX)
      DIMENSION C(28),CNTROX(27),DCVX(27,30)
      DIMENSION AP(102),W(505)
      COMMON AA,AK,BK,IX,MM,L,N,W,AP,PART,HOMO1,BS,HOMO2,HOMO3
      CSUM=0.
      DO 1  I=1,KLT1
    1 CSUM=CSUM+C(I)
      DO 3  I=1,NDIM
      AXIS=0.
      DO 2  J=1,KLT1
      CNTROX(I)=AXIS+C(J)*DCVX(I,J)
      AXIS=CNTROX(I)
    2 CONTINUE
      CNTROX(I)=CNTROX(I)/CSUM
    3 CONTINUE
      RETURN
      END
```

```
      SUBROUTINE SCHECK(K,SUM,NDIM,S)
      DIMENSION S(30)
      DIMENSION AP(102),W(505)
      COMMON AA,AK,BK,IX,MM,L,N,W,AP,PART,HOMO1,BS,HOMO2,HOMO3
      SAVG=0.
      DO 1  L=1,K
    1 SAVG=S(L)+SAVG
      AK=K
      SAVG=SAVG/AK
      SUM=0.
      DO 2  L=1,K
    2 SUM=SUM+(S(L)-SAVG)**2
      ANDIM=NDIM
      SUM=SUM **0.5/ANDIM
      RETURN
      END
```

APPENDIX V. COMPUTER PROGRAM FOR THREE PARAMETERS WITH PERTURBATION WITHOUT NOISE BY QUASILINEARIZATION

```
      EXTERNAL FCT,OUTP,ORDER,CNTROD,SCHECK,SUBNAM
      DIMENSION PRMT(3),Y(4),DERY(4),AUX(6,4),AAP(102)
      DIMENSION BS(102),PART(102),HOMO1(102),HOMO2(102),HOMO3(102)
      DIMENSION PHOY1(5),PHOY2(5),PHOY3(5),PHOY4(5)
      DIMENSION AP(102),W(505),PERT(102)
      DIMENSION DLTVX(27,28),S(30),DCVX(27,30)
      COMMON AA,AK,BK,IX,MM,L,N,M,AP,PART,HOMO1,BS,HOMO2,HOMO3
    1 FORMAT(//,40X,11H ITERATION ,I3)
    2 FORMAT(/,19X,5H TIME,18X,15H SUBJECT MATTER)
    3 FORMAT(16X,F12.4,5X,F12.2,6X,F12.2,6X,F12.2)
    4 FORMAT(F16.8)
    5 FORMAT(4E16.8)
    6 FORMAT(4F16.8)
    7 FORMAT(/,27X,5H PART,16X,6H HOMO1,17X,6H HOMO2)
  101 FORMAT(10I5)
  102 FORMAT(9E8.4)
  103 FORMAT(/16H EVALUATION NO =I5/)
  104 FORMAT(6E13.6)
  105 FORMAT(20X,E18.9,5X,E18.9,5X,E18.9)
  106 FORMAT(/,29X,2HKA,20X,3H KB,21X,3H KB)
      READ(1,6) (PRMT(I),I=1,3)
      READ(1,6) EQUNO,VARIA
      READ(1,6) CC,CP,CG
      READ(1,6) (PHOY1(M),M=1,4)
      READ(1,6) (PHOY2(M),M=1,4)
      READ(1,6) (PHOY3(M),M=1,4)
      READ(1,6) (PHOY4(M),M=1,4)
      READ(1,101)NDIM,NOPT,NDIMP1,MAXNO,METHOD
      READ(1,102)ERROR,SUPLIM
      READ(1,102)((DLTVX(I,J),I=1,NDIM),J=1,NDIMP1)
      READ(1,4) (BS(I),I=1,101)
      READ(1,104) (DCVX(I,1),I=1,NDIM)
      ALPHA=.2
      IY=1
      AA=6.0
      AK=2.0
      BK=0.40
      AP(1)=80.0
    8 JJ=1
      IX=1
      WRITE(3,106)
      WRITE(3,105) AA,AK,BK
   11 WRITE(3,1) JJ
      M=1
      MM=1
      N=1
      NDIM=EQUNO
   12 L=1
```

```
      Y(1)=PHCY1(M)
      Y(2)=PHCY2(M)
      Y(3)=PHCY3(M)
      IF(NDIM-2) 16,16,15
   15 Y(4)=PHCY4(M)
   16 CALL RKGS(PRMT,Y,DERY,FCT,OUTP,NDIM,AUX)
      MM=MM+1
      M=M+1
      IF(M-FGUNC) 12,12,17
   17 IF(IX-10) 28,28,45
   28 IX=IX+1
      N=1
      DO 29 I=1,101
      PART(I)=W(N)
      N=N+1
   29 CONTINUE
      N=102
      DO 30 I=1,101
      HOMO1(I)=W(N)
      N=N+1
   30 CONTINUE
      N=203
      DO 31 I=1,101
      HOMO2(I)=W(N)
      N=N+1
   31 CONTINUE
      IF(NDIM-2) 33,33,32
   32 N=304
      DO 107 I=1,101
      HOMO3(I)=W(N)
      N=N+1
  107 CONTINUE
   33 NDIM=VARIA
      WRITE(3,101)NDIM,NOPT,NDIMP1,MAXNO,METHOD
      WRITE(3,104)ERROR,SUPLIM
      WRITE(3,104)(DCVX(I,1),I=1,NDIM)
      WRITE(3,104)((DLTVX(I,J),I=1,NDIM),J=1,NDIMP1)
      CALL GKCHEN(NDIM,METHOD,MAXNO,ERROR,SUPLIM,DLTVX,DCVX,S,KK)
      WRITE(3,104)S(NDIM+2),(DCVX(I,NDIM+2),I=1,NDIM)
      WRITE(3,104)((DCVX(I,J),I=1,NDIM),J=1,NOPT)
      WRITE(3,104)(S(I),I=1,NOPT)
      WRITE(3,103)KK
      AA=DCVX(1,NDIM+2)
      AK=DCVX(2,NDIM+2)
      IF(NDIM-2) 35,35,111
  111 BK=DCVX(3,NDIM+2)
   35 XX=0.0
      WRITE(3,2)
      IF(NDIM-3) 36,36,38
   36 IF(JJ-1) 50,50,38
   50 DO 37 I=1,101
      AP(I)=PART(I)+AA*HOMO1(I)+AK*HOMO2(I)+BK*HOMO3(I)
      WRITE(3,3) XX,BS(I),AP(I)
      XX=XX+PRMT(3)
   37 CONTINUE
      GO TO 40
```

```
38 DO 39 I=1,101
   AAP(I)=AP(I)
   AP(I)=PART(I)+AA*HOMO1(I)+AK*HOMO2(I)+BK*HOMO3(I)
   PERT(I)=ALPHA*(AP(I)-AAP(I))
   AP(I)=AAP(I)+PERT(I)
   WRITE(3,3) XX,BS(I),AP(I),PERT(I)
   XX=XX+PRMT(3)
39 CONTINUE
40 WRITE(3,106)
   AA=CO*AA
   AK=CP*AK
   IF(NDIM-2) 42,42,41
41 BK=CQ*BK
   WRITE(3,105) AA,AK,BK
   GO TO 44
42 WRITE(3,105) AA,AK
44 JJ=JJ+1
   GO TO 11
45 IY=IY+1
   IF(IY-3) 43,43,43
43 STOP
   END
```

```
      SUBROUTINE RKGS(PRMT,Y,DERY,FCT,OUTP,NDIM,AUX)
      DIMENSION Y(1),DERY(1),A(4),B(4),C(4),PRMT(1),AUX(6,1)
      DIMENSION AP(102),W(505)
      COMMON AA,AK,BK,IX,MM,L,N,W,AP,PART,HOMO1,BS,HOMO2,HOMO3
      X=PRMT(1)
      XEND=PRMT(2)
      H=PRMT(3)
      A(1)=.5
      A(2)=.2928932
      A(3)=1.707107
      A(4)=.1666667
      B(1)=2.
      B(2)=1.
      B(3)=1.
      B(4)=2.
      C(1)=.5
      C(2)=.2928932
      C(3)=1.707107
      C(4)=.5
      DO 3 I=1,NDIM
      AUX(3,I)=0.
    3 AUX(6,I)=0.0
      CALL FCT(X,Y,DERY)
      CALL OUTP(X,Y,DERY)
    9 J=1
   10 AJ=A(J)
      BJ=B(J)
      CJ=C(J)
      DO 11 I=1,NDIM
      R1=H*DERY(I)
      R2=AJ*(R1-BJ*AUX(6,I))
      Y(I)=Y(I)+R2
      R2=R2+R2+R2
   11 AUX(6,I)=AUX(6,I)+R2-CJ*R1
      IF(J-4) 12,15,15
   12 J=J+1
      IF(J-3) 13,14,13
   13 X=X+.5*H
   14 CALL FCT(X,Y,DERY)
      GO TO 10
   15 DO 17 I=1,NDIM
   17 AUX(6,I)=AUX(3,I)
      CALL OUTP(X,Y,DERY)
      IF(X-XEND) 9,16,16
   16 RETURN
      END
```

```
      SUBROUTINE FCT(X,Y,DERY)
      DIMENSION PRMT(1),Y(1),DERY(1)
      DIMENSION AP(102),W(505)
      COMMON AA,AK,BK,IX,MM,L,N,W,AP,PART,HOMO1,BS,HOMO2,HOMO3
      IF(MM-1) 1,1,2
    1 E=1.0
      GO TO 3
    2 E=0.0
    3 ANO=100.
      EXPTM=EXP(-BK*X)
      TERM1=((AA*AP(L))*(1.-(AP(L)*EXPTM/ANO))-AK*AP(L))*E
      TERM2=(Y(1)-E*AP(L))*(AA-((2.*AA*AP(L)*EXPTM)/ANO))-AK
      TERM3=(Y(2)-E*AA)*(AP(L)-(AP(L)*AP(L)*EXPTM/ANO))
      TERM4=(Y(3)-AK)*(-AP(L))
      TERM5=(Y(4)-BK)*((-AA*AP(L)*AP(L))*(-X)*EXPTM/ANO)
      DERY(1)=TERM1+TERM2+TERM3+TERM4+TERM5
      DERY(2)=0.0
      DERY(3)=0.0
      DERY(4)=0.0
      RETURN
      END
```

```
      SUBROUTINE OUTP(X,Y,DERY)
      DIMENSION PRMT(1),Y(1),DERY(1)
      DIMENSION AP(102),W(505)
      COMMON AA,AK,BK,IX,MM,L,N,W,AP,PART,HOMO1,BS,HOMO2,HOMO3
      IF(IX-1) 700,700,701
  700 W(N)=Y(1)
      N=N+1
      GO TO 704
  701 W(N)=Y(1)
      N=N+1
      IF(X-.0249) 704,702,702
  702 L=L+1
  704 RETURN
      END
```

```
      SUBROUTINE GKCHEN(NDIM,METHOD,MAXNO,ERROR,SUPLIM,DLTVX,DCVX,S,K
      DIMENSION DLTVX(27,28),C(28),DCVX(27,30),S(30),CNTROX(27)
      DIMENSION AP(102),W(505)
      COMMON AA,AK,BK,IX,MM,L,N,W,AP,PART,HOMO1,BS,HOMO2,HOMO3
  110 FORMAT(/19H THIS IS NEW METHOD/)
  111 FORMAT(/16H THIS IS SIMPLEX/)
  112 FORMAT(/12H THIS IS BOX/)
  113 FORMAT(/16H ****WARNING****/)
  114 FORMAT(  50H INADEQUATE GIVEN MAX. NO FOR FUNCTION EVALUATION,)
  115 FORMAT(47H INCREASING THE MAXNO OR CHANGING THE STEP SIZE/)
      GO TO (116,117,118),METHOD
  116 JMCHEN=1
      KCHEN=1
      ALPHO=1.0
      BETA=0.5
      COEFF=1.2
      GAMMA=2.0
      WRITE(3,110)
      GO TO 1
  117 JMCHEN=1
      KCHEN=2
      ALPHO=1.0
      BETA=0.5
      GAMMA=2.0
      WRITE(3,111)
      GO TO 1
  118 JMCHEN=NDIM
      ALPHO=1.3
      BETA=0.5
      WRITE(3,112)
    1 J=1
      KK=1
      CALL SUBNAM(NDIM,J,SUPLIM,S,DCVX,KK)
      K=NDIM+JMCHEN
      KLT1=K-1
      DO 3  J=2,K
      DO 2 I=1,NDIM
    2 DCVX(I,J)=DCVX(I,1)+DLTVX(I,J-1)
      CALL SUBNAM(NDIM,J,SUPLIM,S,DCVX,KK)
    3 CONTINUE
    4 M=K
      ALPHA=ALPHO
      CALL ORDER(M,NDIM,S,DCVX)
      DO 5  I=1,KLT1
    5 C(I)=1.
      CALL CNTROD(NDIM,KLT1,C,CNTROX,DCVX)
    6 DO 7  I=1,NDIM
    7 DCVX(I,K+1)=CNTROX(I)+ALPHA*(CNTROX(I)-DCVX(I,K))
      J=K+1
      CALL SUBNAM(NDIM,J,SUPLIM,S,DCVX,KK)
      IF(KK-MAXNO)8,8,36
    8 GO TO (9,9,23),METHOD
    9 IF(S(K+1)-S(1))10,10,23
   10 DO 11 I=1,NDIM
   11 DCVX(I,K+2)=CNTROX(I)+GAMMA*(DCVX(I,K+1)-CNTROX(I))
      J=K+2
```

```
      CALL SUBNAM(NDIM,J,SUPLIM,S,DCVX,KK)
      IF(KK-MAXNO)12,12,36
   12 GO TO (16,13),KCHEN
   13 IF(S(K+2)-S(1))14,14,21
   14 S(K)=S(K+2)
      DO 15 L=1,NDIM
   15 DCVX(L,K)=DCVX(L,K+2)
      GO TO 35
   16 IF(S(K+2)-S(K+1))17,17,21
   17 S(K)=S(K+2)
      DO 18 L=1,NDIM
   18 DCVX(L,K)=DCVX(L,K+2)
      M=K
      CALL ORDER(M,NDIM,S,DCVX)
      CALL SCHECK(K,SUM,NDIM,S)
      IF(SUM-ERROR)37,37,19
   19 CVALUE=2*NDIM-1
      DO 20 I=1,KLT1
      C(I)=CVALUE
   20 CVALUE=2*NDIM-2
      CALL CNTROD(NDIM,KLT1,C,CNTROX,DCVX)
      ALPHA=ALPHO*COEFF
      GO TO 6
   21 S(K)=S(K+1)
      DO 22 L=1,NDIM
   22 DCVX(L,K)=DCVX(L,K+1)
      GO TO 35
   23 IF(S(K+1)-S(K-1))21,21,24
   24 IF(S(K+1)-S(K))25,25,27
   25 S(K)=S(K+1)
      DO 26 I=1,NDIM
   26 DCVX(I,K)=DCVX(I,K+1)
   27 DO 28 I=1,NDIM
   28 DCVX(I,K+1)=CNTROX(I)+BETA*(DCVX(I,K)-CNTROX(I))
      J=K+1
      CALL SUBNAM(NDIM,J,SUPLIM,S,DCVX,KK)
      IF(KK-MAXNO)29,29,36
   29 IF(S(K+1)-S(K))30,30,32
   30 S(K)=S(K+1)
      DO 31 I=1,NDIM
   31 DCVX(I,K)=DCVX(I,K+1)
      GO TO 35
   32 DO 34 J=2,K
      DO 33 I=1,NDIM
   33 DCVX(I,J)=(DCVX(I,1)+DCVX(I,J))/2.
      CALL SUBNAM(NDIM,J,SUPLIM,S,DCVX,KK)
   34 CONTINUE
      IF(KK-MAXNO)35,35,36
   35 CALL SCHECK(K,SUM,NDIM,S)
      IF(SUM-ERROR)37,37,4
   36 WRITE(3,113)
      WRITE(3,114)
      WRITE(3,115)
      GO TO 40
   37 DO 38 I=1,KLT1
   38 C(I)=1.
      CALL CNTROD(NDIM,KLT1,C,CNTROX,DCVX)
      DO 39 I=1,NDIM
   39 DCVX(I,K+1)=CNTROX(I)
```

```
      J=K+1
      CALL SUBNAM(NDIM,J,SUPLIM,S,DCVX,KK)
   40 RETURN
      END
```

```
      SUBROUTINE SUBNAM(NDIM,J,SUPLIM,S,DCVX,KK)
      DIMENSION AP(102),W(505),PART(102),HOMO1(102),BS(102),HOMO3(10
      DIMENSION S(30),DCVX(27,30),X(27),XOPT(27),HOMO2(102)
      COMMON AA,AK,BK,IX,MM,L,N,W,AP,PART,HOMO1,BS,HOMO2,HOMO3
    1 FORMAT(31H THE OPTIMUM FUNCTION VALUE IS E13.6)
    2 FORMAT(6E13.6)
    3 FORMAT(10I4)
      IF(J-1)4,4,5
    4 KCONT=10
      ERR=10.
      GO TO 6
    5 KK=KK+1
    6 DO 7  I=1,NDIM
      X(I)=DCVX(I,J)
    7 CONTINUE
      T1=0.0
      DO 20 I=1,101
      T2=X(1)*HOMO1(I)
      T3=X(2)*HOMO2(I)
      T4=X(3)*HOMO3(I)
   20 T1=T1+(PART(I)+T2+T3+T4-BS(I))**2
      T=T1
      S(J)=T
      IF(J-1) 9,9,11
    9 DO 10 I=1,NDIM
      XOPT(I)=X(I)
   10 CONTINUE
      SOPT=T
      IF(J-1)17,17,12
   11 IF(S(1)-S(J))12,9,9
   12 IF(KK-KCONT)14,13,13
   13 WRITE(3,1)SOPT
      WRITE(3,2)(XOPT(I),I=1,NDIM)
      WRITE(3,3)KK
      KCONT=KCONT+10
   14 IF(S(J)-ERR)15,15,17
   15 WRITE(3,1)SOPT
      WRITE(3,2)(XOPT(I),I=1,NDIM)
      WRITE(3,3)KK
      ERR=ERR*0.1
      GO TO 17
   16 S(J)=SUPLIM
   17 RETURN
      END
```

```
      SUBROUTINE ORDER(M,NDIM,S,DCVX)
      DIMENSION S(30),DCVX(27,30)
      DIMENSION AP(102),W(505)
      COMMON AA,AK,BK,IX,MM,L,N,W,AP,PART,HOMO1,BS,HOMO2,HOMO3
      K=M
      KLT1=K-1
      DO  5 I=1,KLT1
      M=M-1
      DO  4 J=1,M
      IF(S(M+1)-S(J))2,2,4
    2 A=S(M+1)
      S(M+1)=S(J)
      S(J)=A
      DO  3 L=1,NDIM
      B=DCVX(L,M+1)
      DCVX(L,M+1)=DCVX(L,J)
      DCVX(L,J)=B
    3 CONTINUE
    4 CONTINUE
    5 CONTINUE
      RETURN
      END
```

```
      SUBROUTINE CNTROD(NDIM,KLT1,C,CNTROX,DCVX)
      DIMENSION C(28),CNTROX(27),DCVX(27,30)
      DIMENSION AP(102),W(505)
      COMMON AA,AK,BK,IX,MM,L,N,W,AP,PART,HOMO1,BS,HOMO2,HOMO3
      CSUM=0.
      DO 1  I=1,KLT1
    1 CSUM=CSUM+C(I)
      DO 3  I=1,NDIM
      AXIS=0.
      DO 2  J=1,KLT1
      CNTROX(I)=AXIS+C(J)*DCVX(I,J)
      AXIS=CNTROX(I)
    2 CONTINUE
      CNTROX(I)=CNTROX(I)/CSUM
    3 CONTINUE
      RETURN
      END
```

```
      SUBROUTINE SCHECK(K,SUM,NDIM,S)
      DIMENSION S(30)
      DIMENSION AP(102),W(505)
      COMMON AA,AK,BK,IX,MM,L,N,W,AP,PART,HOMO1,BS,HOMO2,HOMO3
      SAVG=0.
      DO 1  L=1,K
    1 SAVG=S(L)+SAVG
      AK=K
      SAVG=SAVG/AK
      SUM=0.
      DO 2  L=1,K
    2 SUM=SUM+(S(L)-SAVG)**2
      ANDIM=NDIM
      SUM=SUM **0.5/ANDIM
      RETURN
      END
```

APPENDIX VI. COMPUTER PROGRAM FOR THREE PARAMETERS WITHOUT NOISE BY NUMERICAL INTEGRATION AND SEARCH

```
      EXTERNAL ORDER,CNTROD,SCHECK,SUBNAM
      DIMENSION BS(101),W(202)
      DIMENSION WW(202)
      DIMENSION DLTVX(27,28),S(30),DCVX(27,30)
      COMMON BS,WW
    2 FORMAT(/,19X,5H TIME,18X,15H SUBJECT MATTER)
    3 FORMAT(16X,F12.6,14X,E18.9,4X,E18.9)
    4 FORMAT(F16.8)
  101 FORMAT(10I5)
  102 FORMAT(9E8.3)
  103 FORMAT(/16H EVALUATION NO =I5/)
  104 FORMAT(6E13.6)
  105 FORMAT(7E10.4)
      XX=0.0
      DLXX=.025
      READ(1,101)NDIM,NOPT,NDIMP1,MAXNO,METHOD
      READ(1,105) ERROR,SUPLIM
      READ(1,102)((DLTVX(I,J),I=1,NDIM),J=1,NDIMP1)
      READ(1,4) (BS(I),I=1,101)
      IY=1
   22 READ(1,105) (DCVX(I,1),I=1,NDIM)
      WRITE(3,101)NDIM,NOPT,NDIMP1,MAXNO,METHOD
      WRITE(3,104)ERROR,SUPLIM
      WRITE(3,104)(DCVX(I,1),I=1,NDIM)
      WRITE(3,104)((DLTVX(I,J),I=1,NDIM),J=1,NDIMP1)
      CALL GKCHEN(NDIM,METHOD,MAXNO,ERROR,SUPLIM,DLTVX,DCVX,S,KK)
      WRITE(3,104)S(NDIM+2),(DCVX(I,NDIM+2),I=1,NDIM)
      WRITE(3,104)((DCVX(I,J),I=1,NDIM),J=1,NOPT)
      WRITE(3,104)(S(I),I=1,NOPT)
      WRITE(3,103)KK
      WRITE(3,2)
      DO 50 I=1,101
      WRITE(3,3) XX,WW(I),BS(I)
      XX=XX+DLXX
   50 CONTINUE
      IY=IY+1
      IF(IY-1) 43,43,43
   43 STOP
      END
```

```
      SUBROUTINE GKCHEN(NDIM,METHOD,MAXNO,ERROR,SUPLIM,DLTVX,DCVX,S,KK
      DIMENSION WW(202)
      DIMENSION BS(101)
      DIMENSION DLTVX(27,28),C(28),DCVX(27,30),S(30),CNTROX(27)
      COMMON BS,WW
  110 FORMAT(/19H THIS IS NEW METHOD/)
  111 FORMAT(/16H THIS IS SIMPLEX/)
  112 FORMAT(/12H THIS IS BOX/)
  113 FORMAT(/16H ****WARNING****/)
  114 FORMAT(  50H INADEQUATE GIVEN MAX. NO FOR FUNCTION EVALUATION,)
  115 FORMAT(47H INCREASING THE MAXNO OR CHANGING THE STEP SIZE/)
      GO TO (116,117,118),METHOD
  116 JMCHEN=1
      KCHEN=1
      ALPHO=1.0
      BETA=0.5
      COEFF=1.2
      GAMMA=2.0
      WRITE(3,110)
      GO TO 1
  117 JMCHEN=1
      KCHEN=2
      ALPHO=1.0
      BETA=0.5
      GAMMA=2.0
      WRITE(3,111)
      GO TO 1
  118 JMCHEN=NDIM
      ALPHO=1.3
      BETA=0.5
      WRITE(3,112)
    1 J=1
      KK=1
      CALL SUBNAM(NDIM,J,SUPLIM,S,DCVX,KK)
      K=NDIM+JMCHEN
      KLT1=K-1
      DO 3  J=2,K
      DO 2 I=1,NDIM
    2 DCVX(I,J)=DCVX(I,1)+DLTVX(I,J-1)
      CALL SUBNAM(NDIM,J,SUPLIM,S,DCVX,KK)
    3 CONTINUE
    4 M=K
      ALPHA=ALPHO
      CALL ORDER(M,NDIM,S,DCVX)
      DO 5  I=1,KLT1
    5 C(I)=1.
      CALL CNTROD(NDIM,KLT1,C,CNTROX,DCVX)
    6 DO 7  I=1,NDIM
    7 DCVX(I,K+I)=CNTROX(I)+ALPHA*(CNTROX(I)-DCVX(I,K))
      J=K+1
      CALL SUBNAM(NDIM,J,SUPLIM,S,DCVX,KK)
      IF(KK-MAXNO)8,8,36
    8 GO TO (9,9,23),METHOD
    9 IF(S(K+1)-S(1))10,10,23
   10 DO 11 I=1,NDIM
   11 DCVX(I,K+2)=CNTROX(I)+GAMMA*(DCVX(I,K+1)-CNTROX(I))
```

```
      J=K+2
      CALL SUBNAM(NDIM,J,SUPLIM,S,DCVX,KK)
      IF(KK-MAXNC)12,12,36
   12 GO TO (16,13),KCHEN
   13 IF(S(K+2)-S(1))14,14,21
   14 S(K)=S(K+2)
      DO 15 L=1,NDIM
   15 DCVX(L,K)=DCVX(L,K+2)
      GO TO 35
   16 IF(S(K+2)-S(K+1))17,17,21
   17 S(K)=S(K+2)
      DO 18 L=1,NDIM
   18 DCVX(L,K)=DCVX(L,K+2)
      M=K
      CALL ORDER(M,NDIM,S,DCVX)
      CALL SCHECK(K,SUM,NDIM,S)
      IF(SUM-ERROR)37,37,19
   19 CVALUE=2*NDIM-1
      DO 20 I=1,KLT1
      C(I)=CVALUE
   20 CVALUE=2*NDIM-2
      CALL CNTROD(NDIM,KLT1,C,CNTROX,DCVX)
      ALPHA=ALPHO*COEFF
      GO TO 6
   21 S(K)=S(K+1)
      DO 22 L=1,NDIM
   22 DCVX(L,K)=DCVX(L,K+1)
      GO TO 35
   23 IF(S(K+1)-S(K-1))21,21,24
   24 IF(S(K+1)-S(K))25,25,27
   25 S(K)=S(K+1)
      DO 26 I=1,NDIM
   26 DCVX(I,K)=DCVX(I,K+1)
   27 DO 28 I=1,NDIM
   28 DCVX(I,K+1)=CNTROX(I)+BETA*(DCVX(I,K)-CNTROX(I))
      J=K+1
      CALL SUBNAM(NDIM,J,SUPLIM,S,DCVX,KK)
      IF(KK-MAXNC)29,29,36
   29 IF(S(K+1)-S(K))30,30,32
   30 S(K)=S(K+1)
      DO 31 I=1,NDIM
   31 DCVX(I,K)=DCVX(I,K+1)
      GO TO 35
   32 DO 34 J=2,K
      DO 33 I=1,NDIM
   33 DCVX(I,J)=(DCVX(I,1)+DCVX(I,J))/2.
      CALL SUBNAM(NDIM,J,SUPLIM,S,DCVX,KK)
   34 CONTINUE
      IF(KK-MAXNC)35,35,36
   35 CALL SCHECK(K,SUM,NDIM,S)
      IF(SUM-ERROR)37,37,4
   36 WRITE(3,113)
      WRITE(3,114)
      WRITE(3,115)
      GO TO 40
   37 M=K
      CALL ORDER(M,NDIM,S,DCVX)
      DO 38 I=1,KLT1
   38 C(I)=1.
```

```
      CALL CNTROD(NDIM,KLT1,C,CNTROX,DCVX)
      DO 39 I=1,NDIM
   39 DCVX(I,K+1)=CNTROX(I)
      J=K+1
      CALL SUBNAM(NDIM,J,SUPLIM,S,DCVX,KK)
   40 RETURN
      END
```

```
      SUBROUTINE SUBNAM(NDIM,J,SUPLIM,S,DCVX,KK)
      DIMENSION S(30),DCVX(27,30),X(27),XOPT(27)
      DIMENSION BS(101)
      DIMENSION Y(1),DERY(1),A(4),B(4),C(4),PRMT(4),AUX(6,6)
      DIMENSION W(202)
      DIMENSION WW(202)
      COMMON BS,WW
    1 FORMAT(31H THE OPTIMUM FUNCTION VALUE IS E13.6)
    2 FORMAT(6E13.6)
    3 FORMAT(10I4)
  107 FORMAT(3F16.4)
      IF(J-1)4,4,5
    4 KCONT=10
      ERR=10.
      GO TO 6
    5 KK=KK+1
    6 DO 7  I=1,NDIM
      X(I)=DCVX(I,J)
    7 CONTINUE
      IF(X(1).GT.12.) GO TO 16
      XXX=0.0
      DLXXX=.025
      Y(1)=50.
      SUM1=0.0
      N=1
      PRMT(1)=0.0
      PRMT(2)=2.499
      PRMT(3)=.025
      Z=PRMT(1)
      XEND=PRMT(2)
      H=PRMT(3)
      A(1)=.5
      A(2)=.2928932
      A(3)=1.707107
      A(4)=.1666667
      B(1)=2.
      B(2)=1.
      B(3)=1.
      B(4)=2.
      C(1)=.5
      C(2)=.2928932
      C(3)=1.707107
      C(4)=.5
      DO 20 I=1,NDIM
      AUX(3,I)=0.
   20 AUX(6,I)=0.0
      ANC=100.
      DATA1=X(1)*Y(1)
      DATA2=(1.-(Y(1)/(ANC*EXP(X(3)*Z))))
      DATA3=X(2)*Y(1)
      DERY(1)=DATA1*DATA2-DATA3
      GO TO 21
   22 M=1
   23 AM=A(M)
      BM=B(M)
      CM=C(M)
```

```
      NDIM=1
      DO 24 I=1,NDIM
      R1=H*DERY(I)
      R2=AM*(R1-BM*AUX(6,I))
      Y(I)=Y(I)+R2
      R2=R2+R2+R2
   24 AUX(6,I)=AUX(6,I)+R2-CM*R1
      IF(M-4) 25,26,26
   25 M=M+1
      IF(M-3) 27,28,27
   27 Z=Z+.5*H
   28 DATA1=X(1)*Y(1)
      DATA2=(1.-(Y(1)/(ANC*EXP(X(3)*Z))))
      DATA3=X(2)*Y(1)
      DERY(1)=DATA1*DATA2-DATA3
      GO TO 23
   26 DO 29 I=1,NDIM
   29 AUX(6,I)=AUX(3,I)
      GO TO 21
   33 IF(Z-XEND) 22,34,34
   21 W(N)=Y(1)
      N=N+1
      IF(N-2) 31,31,32
   31 GO TO 22
   32 GO TO 33
   34 I=1
      DO 35 I=1,101
   35 SUM1=SUM1+(W(I)-BS(I))*(W(I)-BS(I))
      T=SUM1
      S(J)=T
      NDIM=3
      IF(J-1)9,9,11
    9 DO 10 I=1,NDIM
      XOPT(I)=X(I)
   10 CONTINUE
      DO 18 I=1,101
   18 WW(I)=W(I)
      SOPT=T
      IF(J-1) 102,102,12
   11 IF(S(1)-S(J))12,9,9
   12 IF(KK-5) 102,102,101
  101 IF(KK-KCONT) 14,13,13
   13 WRITE(3,1)SOPT
      WRITE(3,3)KK
      WRITE(3,2)(XOPT(I),I=1,NDIM)
      DO 50 I=1,101
      WRITE(3,107) XXX,WW(I)
      XXX=XXX+DLXXX
   50 CONTINUE
      KCONT=KCONT+10
   14 IF(S(J)-ERR)15,15,17
   15 WRITE(3,1)SOPT
      WRITE(3,2)(XOPT(I),I=1,NDIM)
      WRITE(3,3)KK
      ERR=ERR*0.1
      GO TO 17
   16 S(J)=SUPLIM
  102 WRITE(3,1) SOPT
      WRITE(3,2) (XOPT(I),I=1,NDIM)
```

```
      XXX=0.0
      DO 19 I=1,101
      WRITE(3,107) XXX,WW(I)
      XXX=XXX+DLXXX
   19 CONTINUE
      WRITE(3,3) KK
   17 RETURN
      END
```

```
      SUBROUTINE ORDER(M,NDIM,S,DCVX)
      DIMENSION S(30),DCVX(27,30)
      DIMENSION BS(101)
      DIMENSION WW(202)
      COMMON BS,WW
      K=M
      KLT1=K-1
      DO  5 I=1,KLT1
      M=M-1
      DO  4 J=1,M
      IF(S(M+1)-S(J))2,2,4
    2 A=S(M+1)
      S(M+1)=S(J)
      S(J)=A
      DO  3 L=1,NDIM
      B=DCVX(L,M+1)
      DCVX(L,M+1)=DCVX(L,J)
      DCVX(L,J)=B
    3 CONTINUE
    4 CONTINUE
    5 CONTINUE
      RETURN
      END
```

```
      SUBROUTINE CNTROD(NDIM,KLT1,C,CNTROX,DCVX)
      DIMENSION C(28),CNTROX(27),DCVX(27,30)
      DIMENSION BS(101)
      DIMENSION WW(202)
      COMMON BS,WW
      CSUM=0.
      DO 1  I=1,KLT1
    1 CSUM=CSUM+C(I)
      DO 3  I=1,NDIM
      AXIS=0.
      DO 2  J=1,KLT1
      CNTROX(I)=AXIS+C(J)*DCVX(I,J)
      AXIS=CNTROX(I)
    2 CONTINUE
      CNTROX(I)=CNTROX(I)/CSUM
    3 CONTINUE
      RETURN
      END
```

```
      SUBROUTINE SCHECK(K,SUM,NDIM,S)
      DIMENSION S(30)
      DIMENSION BS(101)
      DIMENSION WW(202)
      COMMON BS,WW
      SAVG=0.
      DO 1  L=1,K
    1 SAVG=S(L)+SAVG
      AK=K
      SAVG=SAVG/AK
      SUM=0.
      DO 2  L=1,K
    2 SUM=SUM+(S(L)-SAVG)**2
      ANDIM=NDIM
      SUM=SUM **0.5/ANDIM
      RETURN
      END
```

PART II. SIMULATION AND OPTIMIZATION OF ENVIRONMENT SYSTEMS

INTRODUCTION

A basic problem in the study of life support systems is to establish conditions under which human beings feel thermally comfortable. Since the condition for thermal comfort is influenced by various factors in a complex manner it has been very difficult, if not at all possible, to bring all the factors involved together to study their effects on each other. Fanger [1] has made an attempt to bring many of the factors together and established a fairly general equation for thermal comfort.

The first purpose of this part of the work was to illustrate how the systems techniques could be used to analyze life support system. The second purpose was to study the behavior of Fanger's comfort equation by simulating the feasible region of the comfort equation. The third purpose was to minimize the energy requirement of a typical life support system under the constraint of the comfort equation.

STATEMENT OF PROBLEM

The existing conditions inside and outside a life support system is important for comfortable existence in the system. A study was made of the interaction between these conditions.

Supposed that an equilibrium condition is maintained inside an enclosed area shown in Figure 1. If the outside conditions are different from that of the inside, the incoming air would disturb the equilibrium condition inside. It can happen in four ways:

(1) If outside temperature and relative humidity are higher than those of the inside, the incoming air will give up its heat in the room.

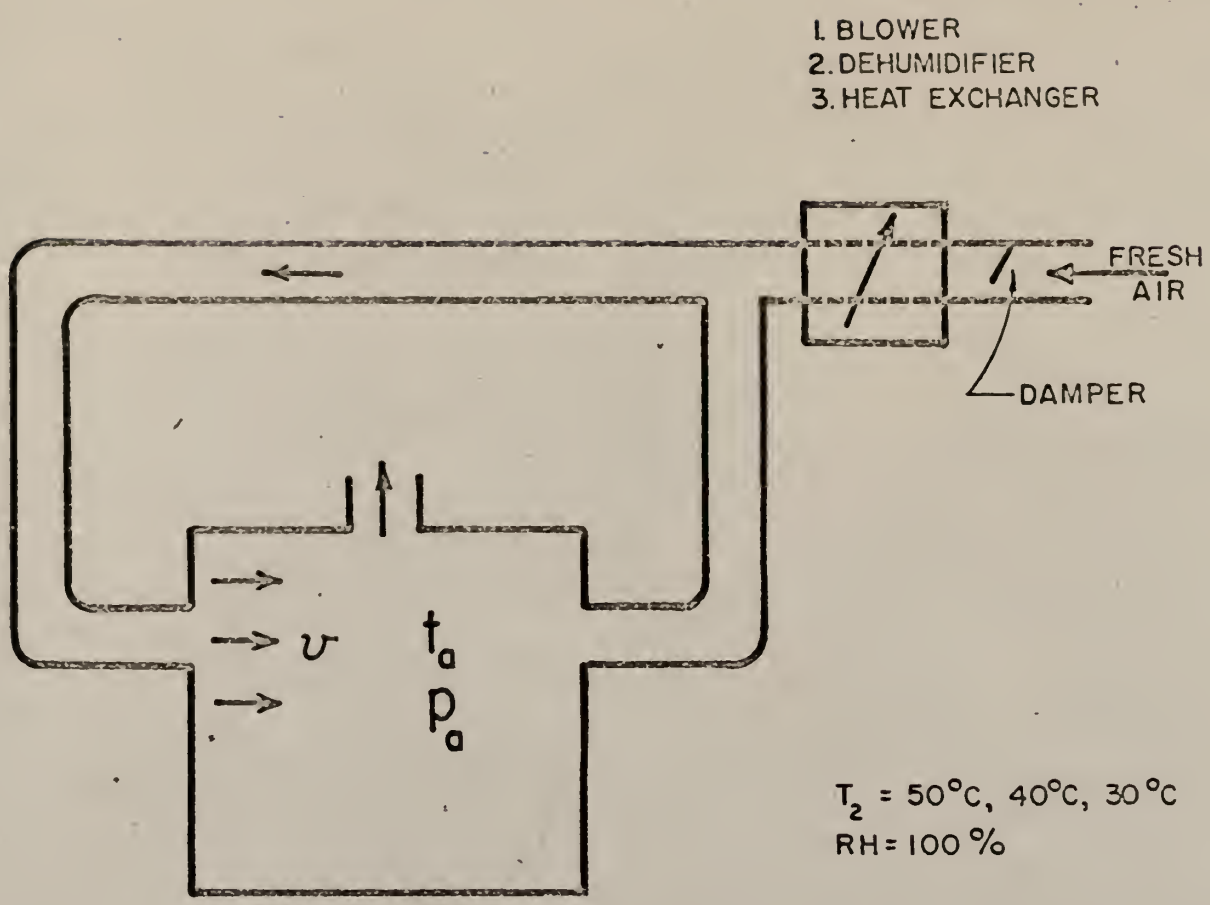

FIGURE 1. THE MODEL

CONDITIONS OF DISTURBANCE:

(1) $T_2 > T_a$; $RH_{out} > RH_{in}$ — GIVES UP HEAT IN THE ROOM.

(2) $T_2 < T_a$; $RH_{out} < RH_{in}$ — ABSORBS HEAT FROM ROOM.

(3) $T_2 > T_a$; $RH_{out} < RH_{in}$

(4) $T_2 < T_a$; $RH_{out} > RH_{in}$

} EITHER GIVES UP OR ABSORBS HEAT IN THE ROOM.

(2) If the outside temperature and relative humidity are lower than those of the inside, the incoming air will absorb heat from the room.

(3) If the outside temperature is higher than the inside temperature but the relative humidity is lower than that of the inside, then the incoming air will either give up or absorb heat in the room depending on the specific instance.

(4) If the outside temperature is lower than that of the inside but the relative humidity is higher than that of the inside, then the incoming air will either give up or absorb heat in the room depending on the specific instance.

In this work only the first situation was considered. Specifically it was considered that the outside conditions are more hazardous than that of the inside and the incoming air bring in heat in three different forms:

(1) Sensible heat (or dry heat) is brought about due to the difference between the outside and the inside temperature. This relationship is shown below.

$$S_1 = f_1(T_2 - t_a) \qquad (1)$$

S_1 = sensible heat in Kcal/hour

T_2 = outside temperature in ^{o}C

t_a = inside temperature in ^{o}C

(2) Latent heat (or wet heat) is brought about by the difference between the outside and the inside partial pressure of water vapour. This relationship is shown below.

$$S_2 = f_2(P_2 - P_a) \qquad (2)$$

S_2 = latent heat in Kcal./hour

P_2 = outside partial pressure of water vapour in mm Hg

P_a = inside partial pressure of water vapour in mm Hg.

(3) Frictional heat which is brought about by the friction in the air duct.

$$S_3 = f_3(\bar{V}(v)) \tag{3}$$

S_3 = frictional heat in Kcal./hour

$\bar{V}$ = air velocity in the duct in meter/sec.

v = air velocity in the room, meter/sec.

Therefore, the total heat brought in is

$$S = S_1 + S_2 + S_3 \tag{4}$$

S = total heat brought in by the incoming air which caused the disturbance of the comfort condition inside.

For a given level of activity and an outside condition of T_2, P_2, the problem was to find the best combination of the room temperature t_a, partial pressure of water vapour in the room, p_a and the room air velocity, v, in meters/second so that the total energy brought in by the incoming air is minimized.

Three different outside conditions and four different levels of activities for males were studied.

In this study the equilibrium condition was defined by Fanger's comfort equation and so, before any optimization was carried out, the equation was thoroughly investigated.

LITERATURE SURVEY

Thermal comfort depends on a number of factors. According to Rholes (personal communication) these factors can be classified into three main categories: (1) Reciprocative Factors which include activity, clothing, exposure and social. (2) Organismic Factors which include age, diet, rhythmicity. (3) Physical Factors which include sound, light, area-volume, radiation, inspired gas, atmospheric pressure, force field, air movement, and temperature-relative humidity (RH).

Numerous studies on the above factors were made and usually at most two parameters were studied at a time. The method was to vary the two parameters under investigation while keeping all other parameters constant.

The effect of environmental conditions was very extensively investigated. Several typical studies are discussed below:

Inouye, in 1953, [6] studied the effects of environments with widely different relative humidities on the partition of heat loss of uniformly and lightly clad men and on their subjective sensations of thermal comfort. The environments were selected to slowly cool the skin without inducing visible sweat or apparent shivering during a period of three hours. He concluded that non-fasting men, lightly clad in uniform suits, showed greater heat loss by evaporation in environments maintained at $80^{\circ}F$, $76^{\circ}F$, or $72^{\circ}F$ with a 30 percent RH than with an 80 percent RH. The effects attributed to relative humidity appeared more readily at the higher environmental temperatures.

The subjects reported that the environments maintained at $76^{\circ}F$ or $72^{\circ}F$ with a 30 percent RH felt thermally the same as one with an 80 percent RH. At the time of entrance into the environment having similar temperatures,

they felt warmer in one with an 80 percent than in one with the 30 percent RH. When the limits of thermal comfort were set between the sensations of very slightly warmer and very slightly cooler, the resting, lightly clad men were thermally comfortable for a period of three hours in environments having temperatures 76°F to 72°F and with 30 to 80 percent RH.

Winslow in 1939 [21] carried out a study of the nude body's physiological reactions and sensations of pleasantness under varying atmospheric conditions. It was an attempt to analyze the influence upon physiological reactions and human comfort of widely varying conditions of air temperature, wall temperature, air movement, and humidity. The fundamental thermodynamic process was described by the equation

$$M + S = E + R + C$$

M = rate of metabolism

S = rate of storage (cooling or heating of body tissues)

E = rate of evaporative heat loss

R = rate of radiative heat loss or gain

C = rate of convective heat loss or gain.

His results showed: (1) metabolism for a given subject remained approximately constant within the range of operative temperature employed, 64 to 100°F--operative temperature was the temperature which represented the net physical effect of a given combination of air and wall temperatures. (2) At a critical operative temperature of 88 to 90°F the heat produced by metabolism (roughly 100 kilogram-calories per hour for subject one was balanced by the heat loss due to evaporation and to radiation plus convection-these two major components accounting for about 50 kilogram-

calories each. Storage was zero; that is, the body tissues showed no change in temperature. (3) As one proceeded to higher operative temperatures, the heat received from the environment due to radiation plus convection increased progressively but was exactly balanced by a similarly progressive increase in evaporative heat loss, so that no positive storage (warming of the body) took place. At an operative temperature of 106°F the body was gaining 106 kilogram-calories from the combined influence of walls and air, and this heat gain plus the metabolic heat produced was balanced by a heat loss of 200 kilogram-calories due to evaporation. (4) Below the critical temperature of 86°F the phenomena were wholly different. Evaporative heat loss here changed but slightly, falling from 40 to 20 kilogram-calories per hour as the operative temperature decreased as a result chiefly of the purely physical factor of decreasing vapour pressure difference between skin and air. In this zone of body cooling, heat loss due to combined influence of radiation plus convection increased progressively. Since this progressively increasing heat loss was not balanced, there was a parallel increase in negative storage (cooling of the body tissues).

Hardy in 1938 (3) measured quantitatively the total heat loss and the proportions due to radiation and convection from men exposed to various atmospheric conditions in the temperature range of 71.6°F to 95°F. Radiation accounted for about 70% of the total loss at 71.6°F and at 78.8°F, but this percentage fell rapidly to zero as skin and air temperatures approached each other. Vaporization dissipated 18% to 30% of the heat at the lower air temperatures but accounted for about 100% at 95°F. Convection remained fairly uniform at about 15% until the air temperature rose above

89.6°F. Convection was significantly increased by slight movements of the body or the air.

The basal metabolism of both naked subjects was level throughout the range of air temperatures from 71.6°F to 95°F.

Nevins in 1966 (16) re-evaluated the conditions for thermal comfort as affected by dry bulb temperature and relative humidity. Seven-Point votes were taken. Nine dry bulb temperatures were: 66, 68, 70, 72, 74, 76, 78, 80, and 82°F at each of eight relative humidity: 15, 25, 35, 45, 55, 65, 75, and 85%. The following were his results: (1) There was a strong linear effect of temperature and a smaller, but yet substantial, linear effect of relative humidity. (2) An interaction effect between temperature and humidity was statistically significant at the 5% probability level.

The effect of air movement was investigated by Winslow (20) in 1938 and by Koch (7) in 1960.

Winslow in 1938 (20) investigated the influence of air movement upon heat losses from the clothed human body. It was concluded that two sorts of air movement were involved--the primary movement produced by the exterior forces at work in the experimental booth itself (due to normal air convection, with or without local fans) and modifications of such movement produced by the inductive influence of the warm body of the subject, or by the interference of the body of the subject with the currents set up by exterior forces. When two subjects were subjected to cool environments for periods of 200 minutes, in this experiment the rectal temperature dropped about a quarter of a degree; skin temperature of the trunk about 32.9°F; of the head, 50°F; of the lower extremities, 35.6°F; and of the upper extremities, 37.4°F. He also found that low initial air movements

were increased by induced air currents due to the warmth of the body. High initial air movements were reduced by the physical obstruction of the body.

Koch (7) in 1960 studied the sensation responses to temperature and humidity under still air conditions in the comfort range. He employed twenty-one subjects who were asked to report their impressions on a number of scales which included thermal sensation, sensation of humidity, sensible perspiration, pleasantness, air motion and sensation of warmth or coolness from surrounding surfaces. Each of these scales was arbitrary. A seven-point scale was used for thermal sensations. His results showed that the line of optimum comfort for both winter and summer was approximately straight and ranged from 77.6°F at 30% relative humidity to 76.5°F at 85% relative humidity. It was only slightly dependent on humidity.

Some studies attempted to establish a comfort zone and two of such studies were discussed below.

Houghten (5) in 1923 employed 130 people to determine the comfort zone. The results pointed to the fact that 64.5 degree Effective Temperature was the comfort line. Effective Temperature was a scale of temperature made up of combinations of temperature and humidity; it was an indication of the relative feeling of warmth. At 58.5° effective temperature, all subjects in the test agreed that the condition was too cold which became the lower boundary. The upper boundary was at 72.5° E. T. There was a rapid rise in comfort from 58.5 to 64.5° E. T. followed by a comparatively gradual fall beyond 64.5° indicating that humans were more sensitive to lower than high temperature. It was also found that if subjects dwelt in the same temperature over prolonged periods of time, they became acclimatized to the condition.

McNall (15), in 1967, determined the thermally neutral temperature and zone for men and women with activity levels resulting in metabolic rates of approximately 600, 800 and 1,000 Btu/hour for the average male subject. Activities and occupations included in 600 Btu/hour were: sitting, moderate arm and leg movements, driving car in traffic, housemaid, typewriting rapidly, ironing, and washing floors; that for 800 British Thermal Unit-Hour (Btu/hour) were: sitting, heavy arm and leg movements standing, moderate work at machine or bench, shoemaker, and walking (3 mph); that for 1000 Btu/hour were: walking about, with moderate lifting or pushing, carpenter, metal-worker, and industrial painter. Seven points were used in the voting of thermal sensation. (Thermal comfort was defined as that condition of mind which expressed satisfaction with the thermal environment; comfort zone or zone of thermal neutrality was the environmental condition where the body is able to maintain a balance between heat production and heat loss without significant changes in any of the readily measurable indices of thermal comfort; thermally neutral temperature was the temperature desired most frequently by the subjects for thermal comfort within a zone of thermal neutrality).

The results indicated that for metabolic rates of 600, 800, and 1000 Btu/hour, the thermally neutral temperatures were 72, 66 and 60^{o}F respectively. Men and women preferred similar thermally neutral temperatures; however, the "comfort zone" for men at each metabolic rate included a wider range of temperatures than were included in the women's "comfort zone". Relative humidities of 25, 45 and 65 had little effect upon men and women's "thermal comfort" at the 600 and 800 Btu/hour (approximately) metabolic rates, but the relative humidity did affect the thermal comfort region for women at

the 1000 Btu/hour (approximately) metabolic rate.

The effect of clothing on the physiological reactions of the human body to varying environmental temperatures was investigated by Gagge (2) in 1938. He found that the gross physiological responses of the clothed body when compared with the nude were broadly identical, and that the skin temperature was the prime factor controlling sensations of thermal pleasantness in both, the hot and cold zone and for both clothed and not clothed bodies.

In 1939 Herrington (4) studied more than just two parameters that influenced thermal comfort at the same time. He brought most of the parameters into an equation for the calculation of the heat exchange of the clothed human body as follows:

$$M \pm S - E = k_v(T_{cl} - T_w) + k_c(T_{cl} - T_a)$$

M = metabolism in kg-cal/hour,

S = net change in total heat content of the body mass expressed in kg-cal/M^2/hour,

E = evaporative loss computed as .58x times the evaporative weight loss in grams/hour,

k_v = constant of radiation exchange per ^oC difference between the average surface temperature of the body and that of the enclosing walls,

T_{cl} = average temperature in ^oC of the exposed skin and clothing surfaces of the body system,

T_w = average temperature of the wall surfaces,

T_a = Average temperature of the ambient air surrounding the body,

k_c = constant of convection exchange per ^oC difference between T_s and T_a.

Substituting values for k_v and k_c into the above equation,

$$M \pm S - E = .75 \times (4 \times 4.92 \times 10^{-8}) \times \frac{T_w^3 + (273 + T_{cl})^3}{2} \cdot$$

$$+ 1.0 \sqrt{v} (T_{cl} - T_a)$$

v = velocity of air movement in cm/sec.

He found a limit of physiological tolerance for heat and cold stress. From previous studies he concluded that a rectal temperature of 25°C (77°F) was near the lower limit of average tolerance and the upper limit of tolerance was between 42.2°C (107.96°F) and 43.5°C (110.3°F).

Fanger (1) in 1967 extended Herrington's study and established a comfort equation, which was thoroughly studied in the simulation part of this work and was later used as a constraint in the optimization of energy.

THE COMFORT EQUATION

Since the comfort equation were used extensively in this work, this equation is reviewed briefly in the following. More detailed discussion can be found in the original reference [1].

The sensation of thermal comfort is closely related to the mean skin temperature and sweat secretation. For each activity level there are certain values of the mean skin temperature and sweat secretion which result in thermal comfort for an individual person. Fanger [1] showed that, under thermal comfort conditions, the mean skin temperature and rate of sweat secretion are related to the activity levels by the following equations.

$$\bar{t}_s = 35.7 - 0.032 \frac{M}{A_{Du}} (1 - \eta) \tag{5}$$

$$\bar{S} = A_{Du}(0.42) \left[\frac{M}{A_{Du}} (1 - \eta) - 50\right] \tag{6}$$

where

$\bar{t}_s$ = average mean skin temperature under comfort conditions, ^{o}C.

$\bar{S}$ = average rate of sweat secretion under comfort conditions, kcal/hr

A_{Du} = Dubois body surface area, m^2

M = metabolic rate, kcal/hr

η = external mechanical efficiency, dimensionless.

The metabolic rate per unit body surface area indicates the activity level of a person. For college-age males, the metabolic rates per unit body surface area at the following four different activity levels are [1]

(a) sedentary: $M/A_{Du} = 52$ kcal/m^2hr

(b) low activity level: $M/A_{Du} = 83$ kcal/m^2hr

(c) medium activity level: $M/A_{Du} = 111$ kcal/m^2hr

(d) high activity level: $M/A_{Du} = 132$ kcal/m^2hr.

If no external work is performed by the subjects, the metabolic rate is equal to the internal heat production rate. However, when the external work is performed, a part of the energy is consumed by this work which has been assumed to have an efficiency η.

Equations (5) and (6) represent the basic conditions for thermal comfort. [1]. Given an activity level, the comfort values for $\bar{t}_s$ and $\bar{S}$ can be obtained by solving simultaneously these two equations. However, to maintain steady state comfort conditions, the heat production rate inside the body must be equal to the heat dissipation or consumption rate which is usually controlled by the environmental conditions. Thus the comfort equation can be obtained by using heat balance and the basic equations, Equations (5) and (6). Under steady state conditions, the heat balance of the body is

internal heat production in the human body − heat loss by evaporation from the skin − heat loss by respiration

= heat loss by conduction through clothing

= heat loss by radiation at the outer surface of the clothing + Heat loss by convection at the outer surface of the clothing (7)

Fanger [1] performed this heat balance calculations and obtained the following equation which must be satisfied for thermal comfort.

$$\frac{M}{A_{Du}}(1-\eta) - 0.35\left[43 - 0.061\frac{M}{A_{Du}}(1-\eta) - P_a\right] - 0.42\left[\frac{M}{A_{Du}}(1-\eta) - 50\right] - 0.0023\frac{M}{A_{Du}}(44 - P_a) - 0.0014\frac{M}{A_{Du}}(34 - t_a)$$

$$= \frac{35.7 - 0.032\, M/A_{Du}\,(1-\eta) - t_{c\ell}}{0.18\, I_{c\ell}}$$

$$= 4.8 \times 10^{-8} f_{c\ell} f_{eff}\left[(t_{c\ell} + 273)^4 - (t_{mrt} + 273)^4\right] + f_{c\ell} h_c (t_{c\ell} - t_a),\ \text{kcal/m}^2\text{h} \qquad (8)$$

where

P_a = partial pressure of water vapor in ambient air, mm of Hg

t_a = air temperature, ^oC

t_{cl} = outer temperature of clothed body, ^oC

I_{cl} = dimensionless overall heat transfer resistance from skin to the outer surface of the clothed body

f_{cl} = ratio of the surface area of the clothed body to the nude body

f_{eff} = ratio of the effective radiation area of the clothed body to the surface area of the clothed body

t_{mrt} = mean radiant temperature, ^oC

h_c = convective heat transfer coefficient, $kcal/m^2hr\ ^oC$.

The products, $A_{Du}\ f_{cl}\ f_{eff}$ and $A_{Du}\ f_{cl}$, represents the effective heat transfer area of the clothed body for radiation and convection respectively. For free and forced convections, the values of h_c had been found to be [1]

$$h_c = 2.05\ (t_{cl} - t_a)^{0.25} \quad kcal/m^2hr\ ^oC \quad \text{(free convection)} \qquad (9)$$

and

$$h_c = 10.4\ v^{1/2} \quad kcal/m^2h^oC \quad \text{(forced convection)} \qquad (10)$$

respectively, where

v = relative air velocity <2.6 m/sec.

It should be noted that Equations (9) and (10) are in agreement with the commonly used formulas for free and forced convections respectively [13].

For a motionless person, the relative air velocity is equal to the

actual air velocity. The mean radiant temperature, in relation to a given person placed at a given point with a given body position and a given clothing, is defined as that uniform temperature of a black enclosure, which gives the same heat loss by radiation from the person as in the actual enclosure under study.

Equation (8) actually containes two separate equations. The first equality relation of Equation (8) can be solved for the outer surface temperature of the clothed body, $t_{c\ell}$, giving rise to the following expression.

$$t_{c\ell} = 35.7 + \frac{M}{A_{Du}} [0.019634 I_{c\ell} + \eta\ (0.10835\ I_{c\ell} + 0.032)]$$

$$- (.063414 I_{c\ell}) P_a - (0.0002 I_{c\ell}) t_a$$

$$- 1.071 I_{c\ell}, {}^{0}C \qquad (11)$$

For simplicity, let

$$0.019634\ I_{c\ell} + \ (0.10835\ I_{c\ell} + 0.032) = \alpha \qquad (12)$$

Equating the left hand side of the first equality sign in Equation (8) to the right hand side of the second equality sign of the same equation and using Equations (11) and (12), we obtain

$$\frac{M}{A_{Du}} (1-\eta) - 15.05 + 0.0213 \frac{M}{A_{Du}} (1-\eta) + 0.35\ P_a$$

$$- 0.42 \frac{M}{A_{Du}} (1-\eta) + 21 - 0.1012 \frac{M}{A_{Du}} + 0.0023\ P_a - 0.0476 \frac{M}{A_{Du}}$$

$$+ 0.0014 t_a$$

$$= 4.8 \times 10^{-8} f_{c\ell} f_{eff} [(\alpha \frac{M}{A_{Du}} - 0.063414 I_{c\ell} P_a - 0.0002 I_{c\ell} t_a$$

$$-1.071 I_{c\ell} + 308.7)^4 - (t_{mrt} + 273)^4]$$

$$+ f_{c\ell} h_c (35.7 - \alpha \frac{M}{A_{Du}} - 0.063414 P_a$$

$$- (1 + 0.0002 I_{c\ell}) t_a - 1.071 I_{c\ell}), \text{ kcal/m}^2\text{h} \qquad (13)$$

The following assumptions were made by Fanger [1] in arriving at the above final form of the heat balance equation.

(1) The mean skin temperature, $\bar{t}_s$, and the internal body temperature are important parameters for thermal comfort. The mean skin temperature layes between 27^oC and 37^oC

$$27^oC < \bar{t}_s < 37^oC$$

(2) The heat of vaporization of water at 35^oC is equal to 575 kcal/kg.

Fanger [1] used the following conditions in his experiments,

(1) For each activity level the temperature of air, t_a, was maintained equal to the mean radiant temperature

$$t_a = t_{mrt}.$$

(2) The relative humidity was maintained at 45%.

(3) The external mechanical efficiency of the body, η, was maintained at zero, i.e.

$$\eta = 0.$$

In the present study it was assumed that the convective heat loss was by forced convection only. This implied that the value of convective heat

transfer coefficient, h_c, was given by equation (10).

Since there was a transition zone between free and forced convection, the lower limit of the applicability of Equation (1) was not clearly defined. However, it was found in practical calculations that the lower limit of Equation (10) was approximately 0.1 m/s [1]. This approximation was adopted in this work. Thus the value of v was restricted to the range

$$0.1 < v < 2.6 \tag{14}$$

Taking the above experimental conditions and the assumptions into consideration, the comfort equation, Equation (13) became

$$0.4525 \frac{M}{A_{Du}} + 0.3523 P_a + 0.0014 t_a + 5.95$$

$$= 4.8 \times 10^{-8} f_{c\ell} f_{eff}[(-0.6314 I_{c\ell} P_a - 0.0002 I_{c\ell} t_a$$

$$+ 308.7 + 0.019634 I_{c\ell} \frac{M}{A_{Du}} - 1.071 I_{c\ell})^4 - (t_a + 273)^4]$$

$$+ 10.4 f_{c\ell} \sqrt{v} [-0.063414 P_a - (1 + .0002 I_{c\ell}) t_a$$

$$+ 35.7 + 0.019634 I_{c\ell} \frac{M}{A_{Du}} - 1.071 I_{c\ell}], \text{ kcal/m}^2\text{h} \tag{15}$$

This comfort equation contained the following variables.

$$I_{c\ell}, f_{c\ell}, \frac{M}{A_{Du}}, f_{eff}, v, t_a, P_a .$$

However, in most practical situations in life support systems, only the thermal environmental variables P_a, t_a, and v are controlled, and so other variables, namely, M/A_{Du}, $I_{c\ell}$, $f_{c\ell}$, and f_{eff} were considered as parameters in the present study.

SIMULATION OF COMFORT EQUATION [12]

The values for the parameters, M/A_{Du}, I_{cl}, f_{cl}, and f_{eff}, were furnished by the Institute of Environmental Research, Kansas State University and are tabulated in Table 1. Four types of activities for males were considered. There were total four sets of parameter values for $\frac{M}{A_{Du}}$, I_{cl}, f_{cl}, f_{eff}.

With the assumption that $\frac{M}{A_{Du}}$, I_{cl}, f_{cl}, and f_{eff} are constants for each type of activity, the comfort equation can be written as

$$A + CP_a + Dt_a + 5.95 = E[(-FP_a - Gt_a + W)^4 - (t_a + 273)^4]$$

$$+ X\sqrt{v}\,(-YP_a - Zt_a + U) \qquad (16)$$

where

$$A = 0.4525\,\frac{M}{A_{Du}}$$

$$C = 0.3523$$

$$D = 0.0014$$

$$E = 4.8 \times 10^{-8}\, f_{cl}\, f_{eff}$$

$$F = 0.063414\, I_{cl}$$

$$G = 0.0002\, I_{cl}$$

$$W = 308.7 + 0.019634 I_{cl}\,\frac{M}{A_{Du}} - 1.071 I_{cl}$$

$$X = 10.4\, f_{cl}$$

$$Y = 0.063414$$

$$Z = 1 + 0.0002 I_{cl}$$

$$U = 35.7 + 0.019634 I_{cl} \frac{M}{A_{Du}} - 1.071 I_{cl}$$

It can be seen from Table I that parameters I_{cl} and f_{cl} are the same for all types of activities and f_{eff} changes only for sedentary levels. Thus,

$$F = .0380484$$

$$G = 0.00012$$

$$X = 11.44$$

$$Z = 1.00012$$

The values of A, E, W, and U are different for different types of activities.

Examination of Equation (16) reveals that it depended on the fourth powers of t_a and P_a, but only depended on the square root of v. Thus, the best way to simulate this equation was to assume values for t_a and P_a, and then calculated v from Equation (16). Thus

$$v = \left| \frac{A + CP_a + Dt_a + 5.95 + E[(-FP_a - Gt_a + W)^4 - (t_a + 273)^4]}{X(-YP_a - Zt_a + U)} \right|^2$$

$$= \left| \frac{\text{DATA 1} - \text{DATA 2}}{\text{DATA 3}} \right|^2 \qquad (17)$$

Equation (17) was simulated on an IBM 360/50 computer. The computer flow diagram is shown in Figure 23. Some typical computational results are shown in Figures 2 through 5 where four typical metabolic rates listed in Table 1 were used.

The peculiar behavior of these figures can be attributed to the characteristics of Equation (17). Mathematically, Equation (17) has two limits. The lower limit was zero, which occurs when the numerator is equal to zero, and the upper limit is infinite, which occurs when the denominator is equal to

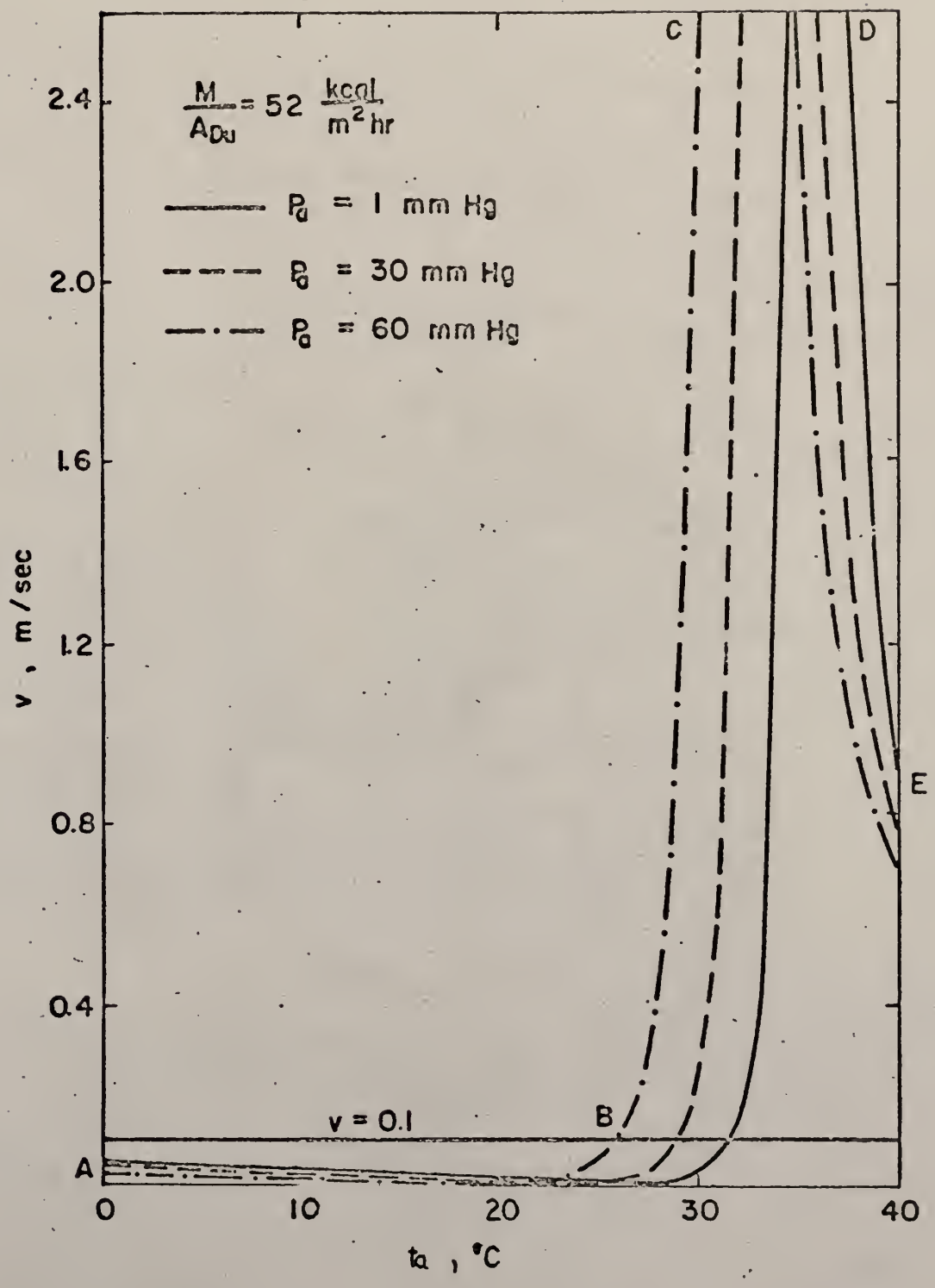

Figure 2. Simulation of comfort equation.

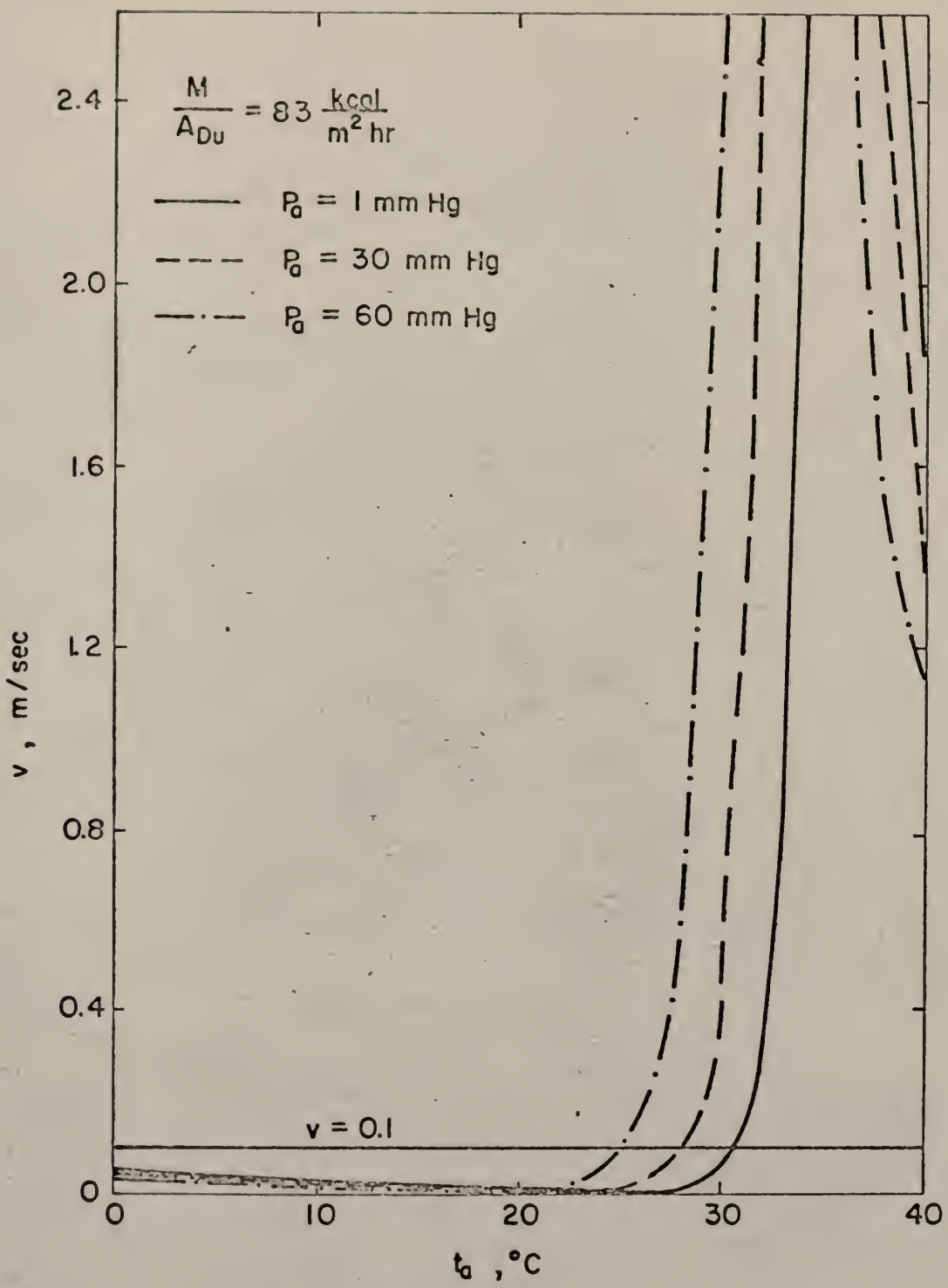

Figure 3. Simulation of comfort equation.

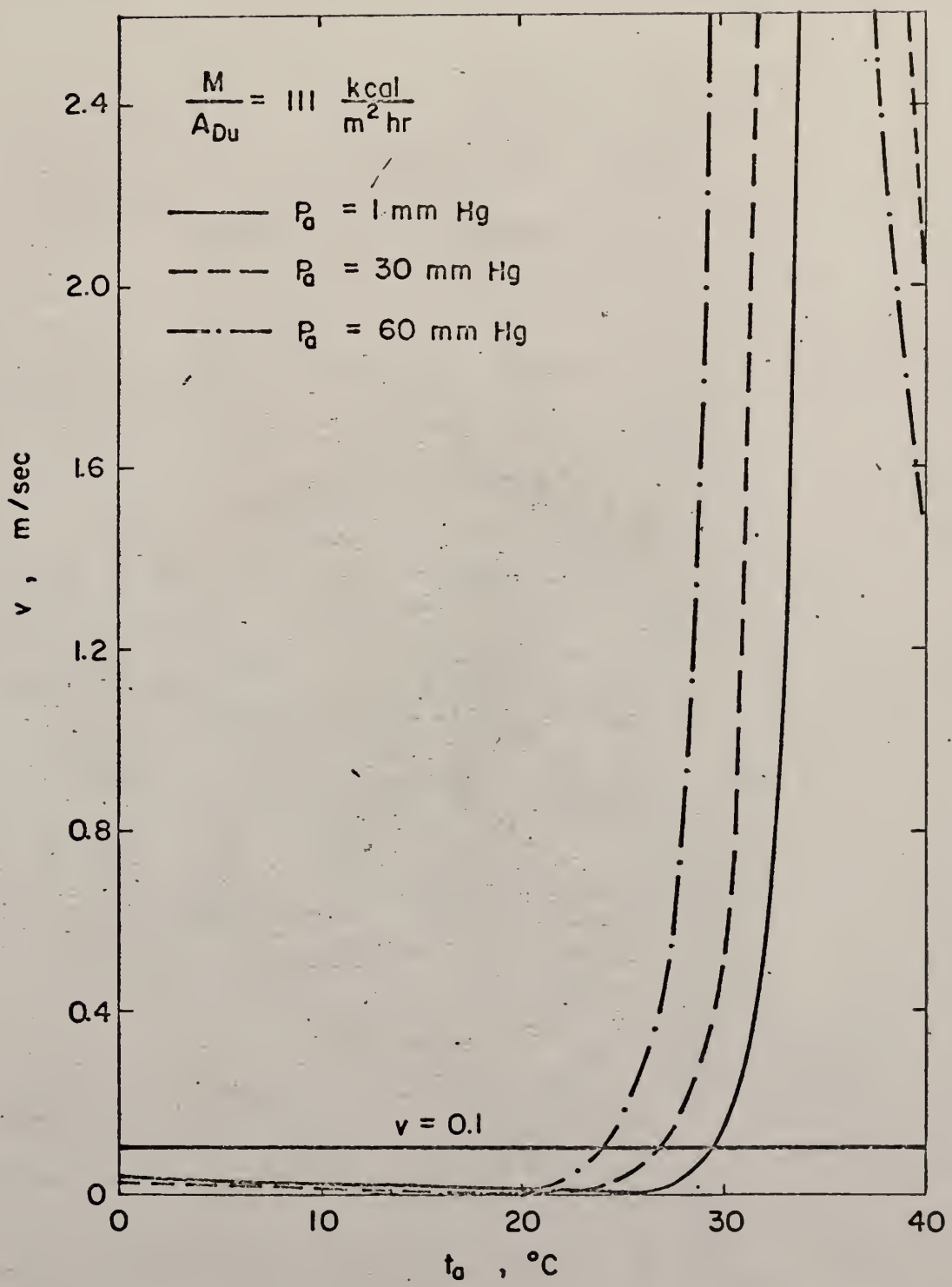

Figure 4. Simulation of comfort equation.

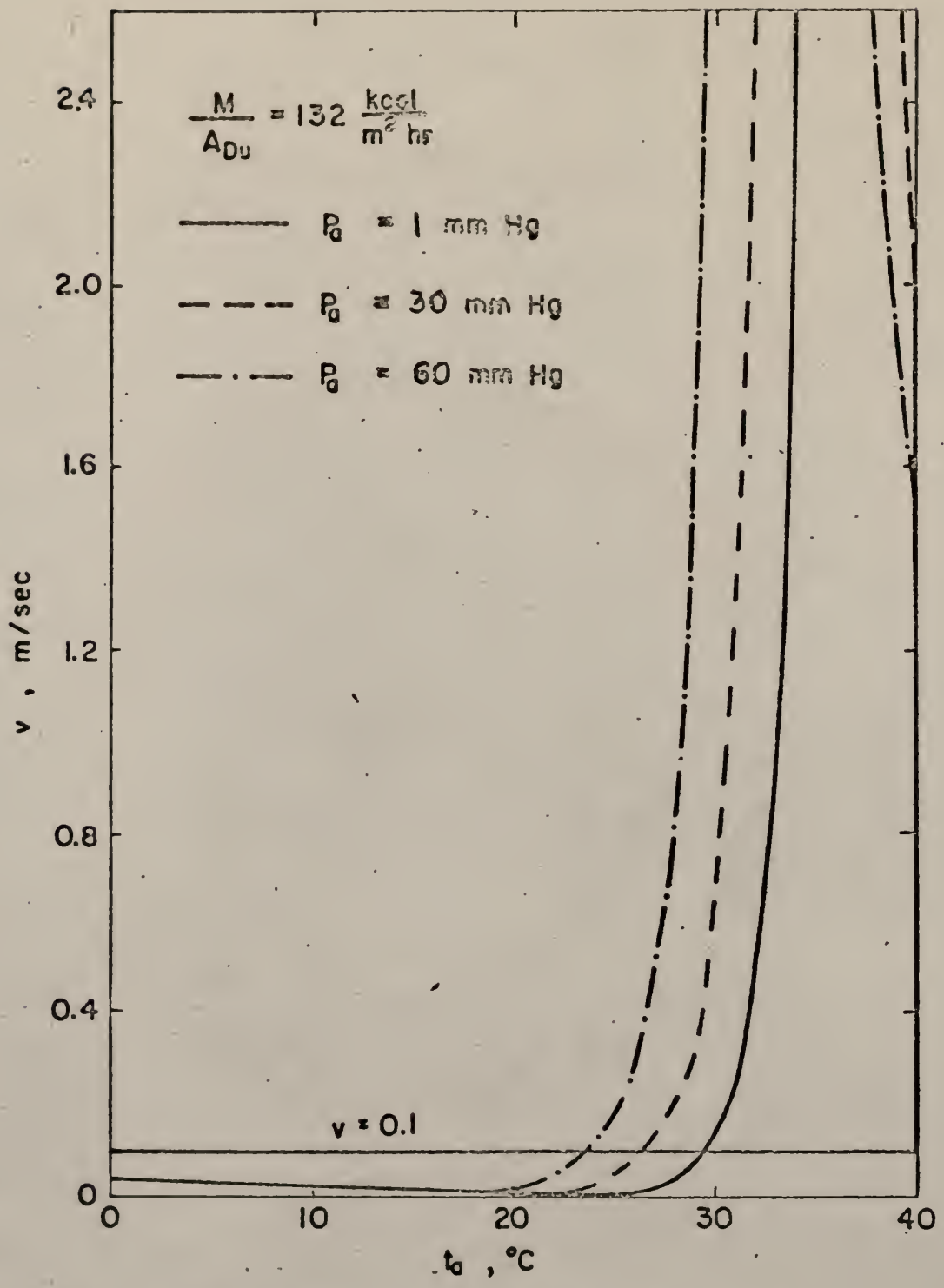

Figure 5. Simulation of comfort equation.

Table 1. Values of Different Parameters

	type of activity	M/A_{Du} kcal/m^2hr	I_{cl}	f_{cl}	f_{eff}
male	sedentary	52	.6	1.1	.65
	low	83	.6	1.1	.75
	medium	111	.6	1.1	.75
	high	132	.6	1.1	.75

zero. These two limits are shown clearly in Figures 2 through 5. Obviously, the comfort equation is feasible only in the region represented by the segment BC (see Figure 2). The feasible regions for P_a = 1 mm Hg, under various different activity levels, are listed in Table 2.

The segments AB and DE are unreasonable regions. The segment AB is infeasible because forced convection has been assumed in establishing Equation (17) and thus the relative velocity of air must be larger than 0.1 m/sec. It should be emphasized that the comfort equation is also applicable for free convection, provided that Equation (9) is used. However, for free convection the relative velocity of air, v, does not appear in the comfort equation.

It is of practical interest to obtain the upper and lower mathematical limits of Equation (17). At the upper limit, where $v \to \infty$, we have

$$X(-YP_a - Zt_a + U) = 0 \tag{18}$$

At the lower limit, where v = 0, we have

$$A + CP_a + Dt_a + 5.95 + E[(-FP_a - Gt_a + W)^4 - (t_a + 273)^4] = 0 \tag{19}$$

By solving Equations (18) and (19), the mathematical upper and lower limits were obtained respectively. The results are shown in Figures 6 and 9.

Equation (18) could be solved easily. However, Equation (19) is a fourth order equation in P_a and t_a and could not be solved easily. Therefore, the Newton-Raphson method was employed to solve Equation (19) numerically. The method was described in Appendix I and the computer flow diagram for this procedure is shown in Figure 22.

Table 2. Feasible Range of t_a, P_a = 1 mm Hg

M/A_{Du} kcal/m^2hr	feasible range of temperature, ^{o}C
52	$31.6 \leq t_a \leq 34.2$
83	$30.6 \leq t_a \leq 34.1$
111	$29.4 \leq t_a \leq 39.9$
132	$28 \leq t_a \leq 33.6$

The physical limits imposed on the comfort equation are given by Equation (14). With these physical limits of v = 0.1 and v = 2.6, Equation (17) could again be solved for P_a as a function of t_a by the Newton-Raphson method.

Results of these calculations were also shown in Figures 6 and 9.

Since Equation (19) is a fourth-order equation, four values of P_a were obtained for each value of t_a. It is worth examining all four roots for feasibility. Equation (19) can be rewritten as

$$f(P_a, t_a) = A + CP_a + Dt_a + 5.95 + E[(-FP_a - Gt_a + W)^4 - (t_a + 273)^4] \quad (20)$$

With $t_a = 20^{\circ}C$, values of the function f had been calculated as a function of P_a. However, it was found that all roots except one are not within the following range of P_a.

$$0 \leq P_a \leq 60 \text{ mm Hg}$$

In fact, no root had been found to exist even within the range of $-60 \leq P_a \leq 0$, which was obviously physically impossible. Thus, Equation (19) only has one feasible root as shown in Figures 6 and 9. The 60 mm HG for the upper limit of P_a was chosen arbitrarily. As can be seen from Figures 6 through 9 P_a = 60 mm Hg is not physically feasible.

Optimization of Comfort Condition:

In this work the energy which must be removed to attain comfort condition in a life support system within an enclosed system was minimized. Other topics of interest such as minimizing the cost of the system, the weight of the equipment required to attain comfort conditions or the

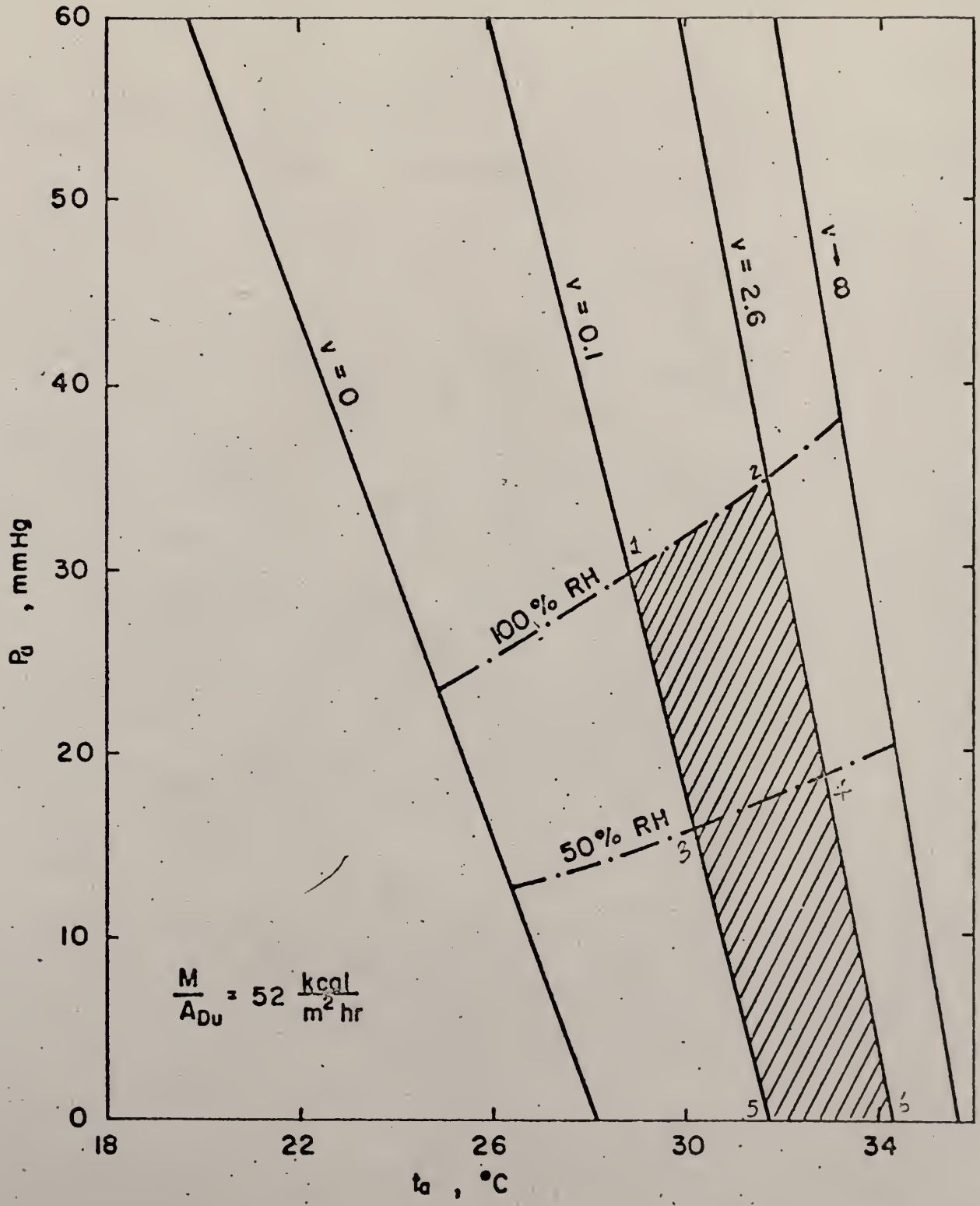

Figure 6. Feasible region of the comfort equation.

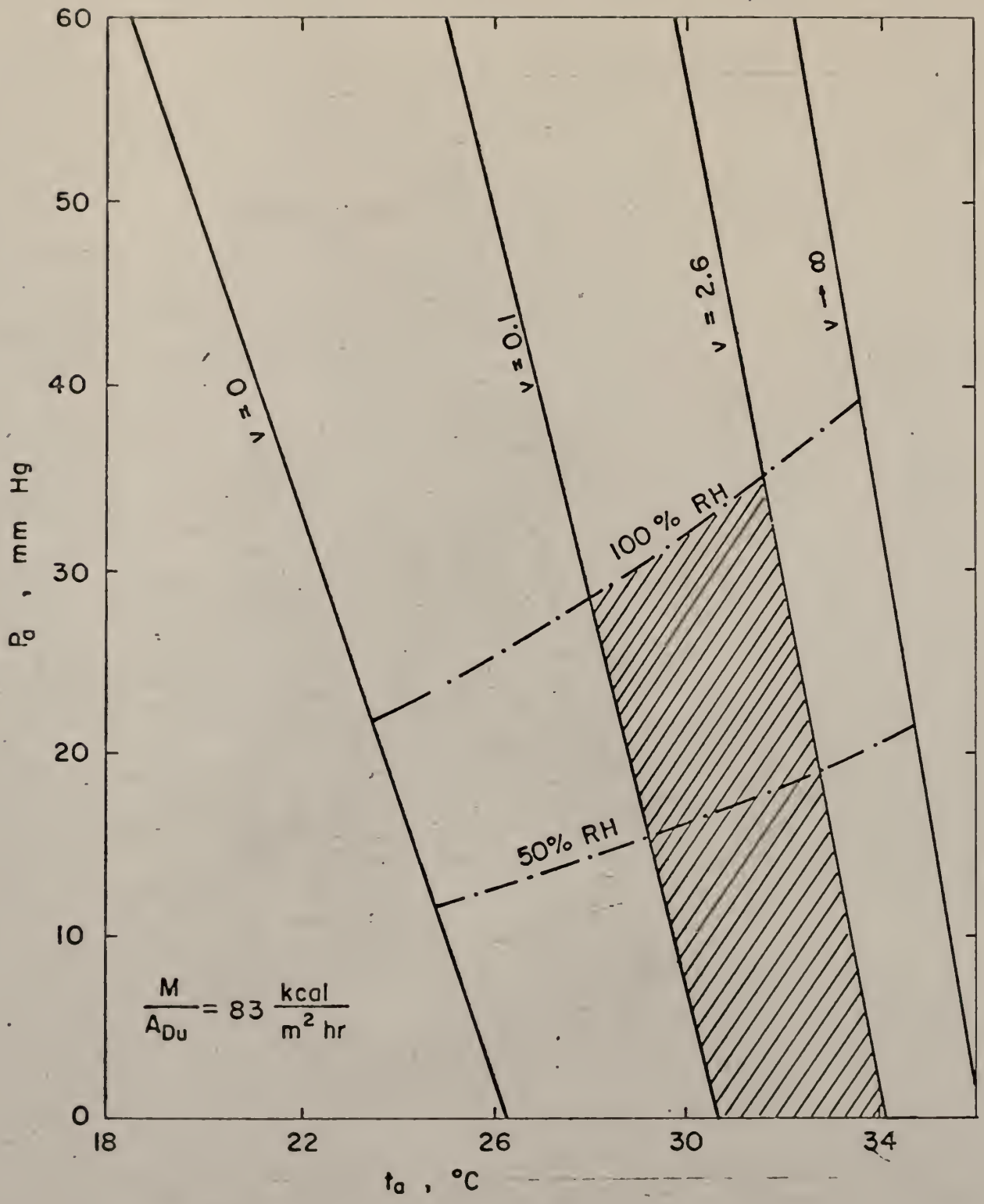

Figure 7. Feasible region of the comfort equation.

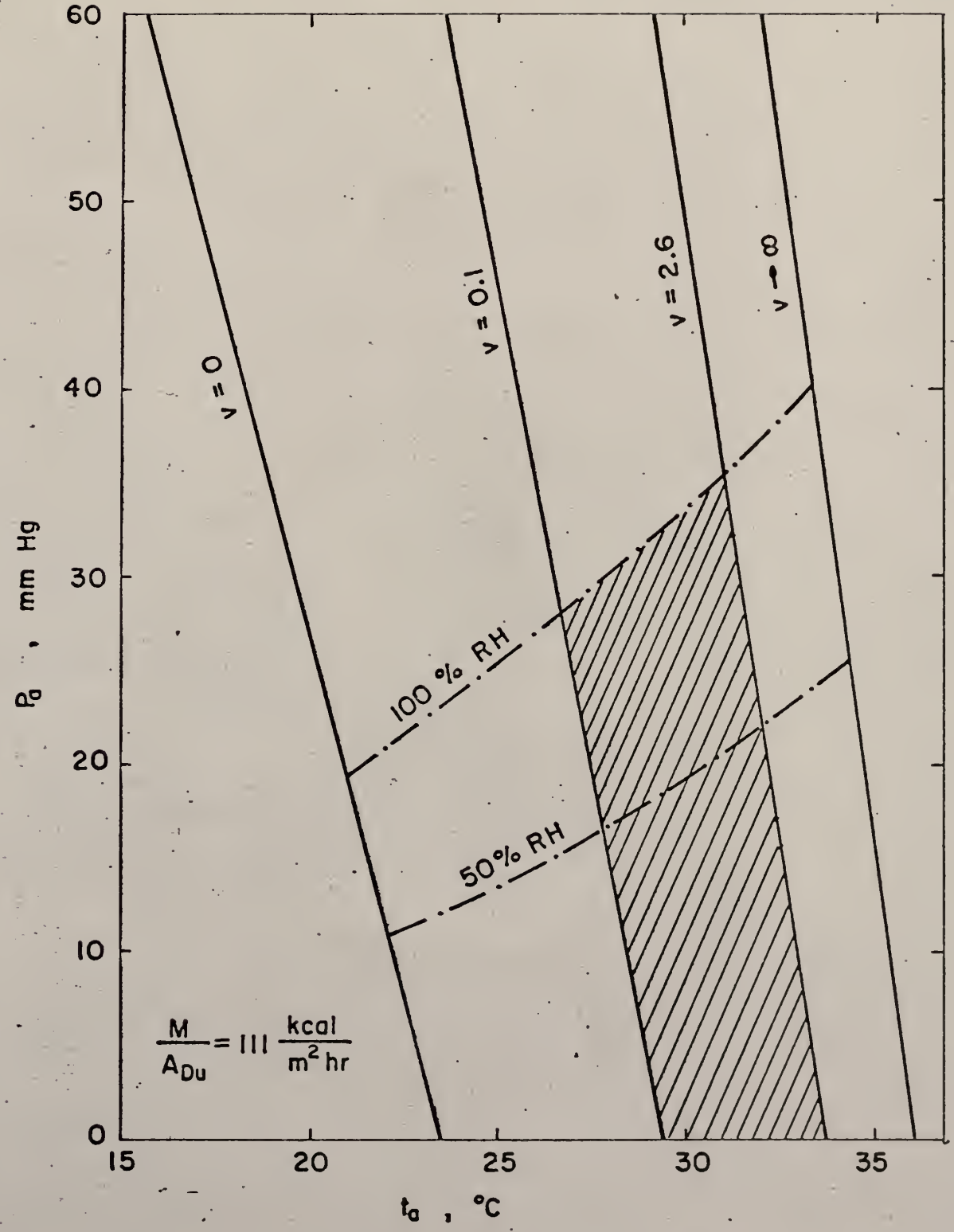

Figure 8. Feasible region of the comfort equation.

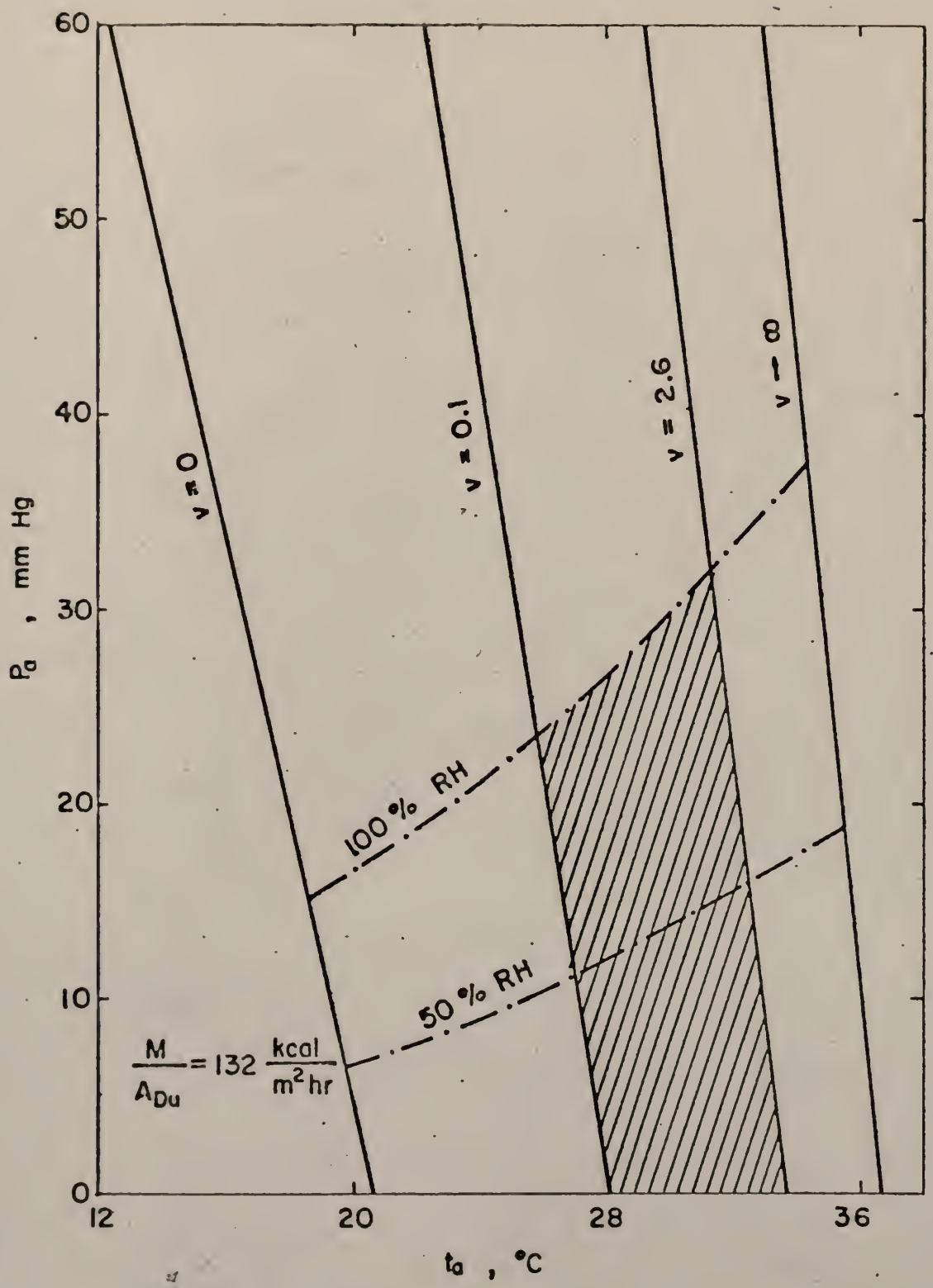

Figure 9. Feasible region of the comfort equation.

maximization of the stability of the system can not be successfully investigated without thoroughly understanding the energy requirements of the system.

The optimization of comfort condition was based on the model shown in Figure 1. The enclosed volume was 3 x 4 x 5 meters [18]. The cross-sectional area perpendicular to the direction of the air flow was 3 x 4 meters. The length and diameter of the duct was 20 meters and .458 meter respectively. It was so designed that only one person was working inside and 283 liters per minute (10 cu. ft. per min.) of fresh air were required.

Three outside conditions were considered: 50° C, 40° C, and 30° C with relative humidity (RH) equal to 100% in all cases. These values were chosen arbitrarily. Extreme conditions were considered to ensure a more hazardous outside conditions so that the incoming air would only give up heat. The air in the enclosure was assumed to be incompressible and completely mixed.

In the Statement of the Problem it was mentioned that the energy brought in by the incoming air could be classified as (1) the sensible heat of air and its vapour content; (2) the latent heat of the water vapour and (3) the frictional heat. Each of the three forms of energy would be analyzed separately before they were combined to form the objective function.

VI-A. PRELIMINARY CALCULATIONS

Three general terms--saturated vapour pressure, specific volume of air and mass rate of air flow were studied first before computing for the energies.

1. Computation of saturated vapour pressure

Saturated vapour pressure was needed in the computation of energy. Therefore, it was desirable to formulate an empirical equation which could be used to obtain the saturated vapour pressure at any given temperature.

A few values of saturated vapour pressure for the corresponding temperatures are tabulated below [17] and their relationships are plotted in Figure 10.

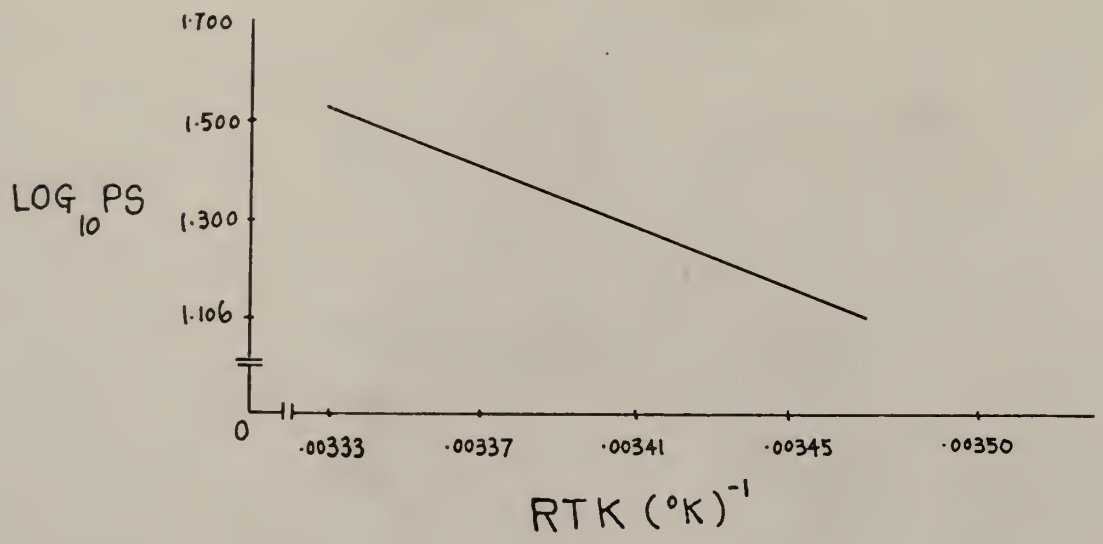

Fig. 10. Relationship of temperature, ^{o}K, and saturated vapour pressure, mm Hg.

Since $\log_{10}$ PS is linearly related to the temperature, their relationship can be expressed as follows:

$$\log PS = a + b(RTK) \tag{21}$$

TABLE 3. RELATIONSHIP OF TEMPERATURE AND SATURATED VAPOUR PRESSURE

TEMPERATURE ($t^{\circ}C$)	SATURATED VAPOUR PRESSURE (PS in mm Hg)	LOG_{10}(SATURATED VAPOUR PRESSURE)(LOG_{10} PS)	$\frac{1}{273+t^{\circ}C}$ (RTK)
15	12.788	1.1060	.00347
20	17.535	1.2440	.003415
25	23.756	1.3755	.003355
30	31.824	1.5030	.00333
35	42.175	1.6250	.00325

Equation (21) describes the linear relationship between RTK and $\log_{10}$ PS. To solve for a and b any two points on the straight line could be used. In this instance the two points used were: RTK = 00847, $\log_{10}$ PS = 1.1060 ($t = 15^{o}$ C) and RTK = .00333, $\log_{10}$ PS = 31.824 ($t = 30^{o}$C).

The above values were substituted into equation (21) to obtain the following two equations.

$$\log_{10} 12.788 = a + b(.00347) \tag{23}$$

$$\log_{10} 31.824 = a + b(.00333) \tag{23}$$

Equation (23) was subtracted from equation (22) giving rise to

$$\log_{10} 12.788 - \log_{10} 31.828 = b(00347 - .00333)$$

$$\log_{10} \frac{12.788}{31.828} = b(.00014)$$

Converting $\log_{10}$ to $\log_{e}$, the following equation was obtained

$$\ln \frac{12.788}{31.828} = b(.00014)\ \ln 10$$

$$b = \frac{\ln 12.788 - \ln 31.828}{(.00014)\ln 10}$$

$$= -2303.81$$

Substituting b into equation (22), a was given as follows

$$a = \log_{10} 12.788 - (-2303.81)(.00347)$$

$$= 9.11$$

Substituting the values of a and b into equation (21), $\log_{10}$PS was obtained

$$\log_{10} PS = 9.11 - 2303.81(RTK)$$

Converting $\log_{10}$ to $\log_e$, the following equation was obtained

$$\ln PS = 20.98 - 5307.02\ (RTK) \tag{24}$$

It was found that in the temperature range of $8^{o}C < t < 36^{o}C$ Equation (24) gives the saturated vapour pressure at any temperature. The relative humidity (RH) at a specific temperature is equal to the partial pressure of water vapour (Pa) at that temperature divided by the saturated vapour pressure at the same temperature. This relationship is expressed as follows:

$$RH = \frac{Pa}{Ps} \tag{24a}$$

2. Computation of specific volume of air.

The specific volume of air was computed as a function of temperature, ^{o}K and vapour partial pressure. This specific volume of air was needed in the computation of mass rate of air flow which was in turn required in the computation of energy. From Dalton's law:

$$V_{sp} = \frac{R(Tk)}{P}$$

V_{sp} = specific volume of dry air in liter/gm.

R = constant

Tk = temperature in ^{o}K $(273 + t^{o}C)$

P = pressure of dry air in mm Hg

and

$$P = (760-P_v) \text{ mm Hg}$$

P_v = Vapour Partial Pressure at t^oC

$$V_{sp} = \frac{(62.361)(Tk)}{(760-P_v)(29)} \quad \text{liter/gram} \tag{25}$$

where 29 was the molecular weight in grams per gm-mole of air.

3. Computation of mass rate of air flow

Mass rate of air flow was formulated as a function of the volumetric flow rate and the specific volume of air as shown below.

$$M = \frac{Q}{V_{sp}} \tag{26}$$

M = mass rate of air flow in gm/hr

Q = volumetric flow of air in liter/hr.

Thus, the mass rate of incoming air is

$$M_2 = \frac{600 \frac{\text{cuft}}{\text{hr}} \times 28.32 \frac{\text{liters}}{\text{cuft}}}{V_{sp} \frac{\text{liter}}{\text{gram}}} \quad \text{gm. per hr.} \tag{26}$$

V_{sp} could be obtained from equation (25).

4. Computation of sensible heat.

Sensible heat or dry heat is due to the difference between the outside and inside temperatures. Two components are involved in the sensible heat--the air and its water vapour content. The increase in the sensible heat in an enclosed area is due to the difference in temperature between the

outside air and its water vapour content, and the inside air and its water vapour content. This relationship is expressed as follow

$$\text{Sensible heat } (SS_1) = M_2 \times CS_2 \times \frac{(T_2 - t_a}{1000} \text{ Kcal./hr.}$$

CS_2 = specific heat of outside air and water content in cal/gm^{o}C

T_2 = outside air temperature in ^{o}C

t_a = room air temperature in ^{o}C

The sensible heat brought in by the incoming air is a function of the incoming air's mass rate, specific heat of the air and its water content and the difference between the temperature of outside air and room air.

For ordinary air temperature the specific heats of dry air and water vapour can be taken as 0.238 and 0.46 cal/gm^{o}C respectively. Thus, the specific heat of air is given as below

$$CS_2 = 0.238 + 0.46\ W_2 \quad \text{cal/gm}^{o}\text{C}$$

where

W_2 = outside molal (absolute) humidity in gm. of water/gm. of air

Humidity is defined as the number of pounds of water in one pound of dry air. Thus, in a mixture of dry air and water vapour if the total pressure is fixed, then the humidity is a function of the partial pressure of water vapour. If the partial pressure of the water vapour is designated as Pa, then the molal ratio of water vapour to dry air at one atmosphere is Pa/(1-Pa). Since the molecular weights of dry air and water are 29gms./gm and 18 gms./gm-mole respectively, the humidity (W) became

$$W = \frac{18P_a}{29\ (1 - P_a)} \quad \text{gm. of water gm. of air}$$

The humidity of outside air is

$$W_2 = \frac{18\ P_{a2}}{29(760 - P_{a2})} \frac{\text{gm. of water}}{\text{gm. of air}} \tag{27a}$$

where

P_{a2} = outside vapour partial pressure in mmttg

Similarly, the humidity in the room is

$$W_1 = \frac{18\ P_a}{29\ (760 - P_a)} \frac{\text{gm. of water}}{\text{gm. of air}} \tag{27b}$$

From equation (27a) the specific heat of outside air and water content is

$$CS_2 = 0.238 + 0.46\ [\frac{18\ P_{a2}}{29(760 - P_{a2}}]\ \frac{\text{cal.}}{\text{gm.}^{o}C} \tag{27c}$$

and equation (27) become

$$\text{Sensible heat (SS.)} = M_2 \times \left\{0.238 + 0.46\ [\frac{18\ P_{a2}}{29(760 - P_{a2})}]\right\} \times \frac{T_2 - t_a}{1000}$$

Kcal

5. Computation of latent heat

Latent heat is also called wet heat and it is due to the difference in water vapour between the outside and inside air. The increase in the latent heat in the room brought in by the incoming air is due to the

difference in humidity between the outside and inside air. This relationship is expressed as follow:

$$\text{Latent heat } (SS_2) = M_2 x (W_2 - W_1) \times \frac{575}{1000} \text{ Kcal. per hr.} \qquad (28)$$

M_2, W_2, W_1 could be obtained from equations (26), (27a) and (27b) respectively.

6. Computation of friction heat.

As incoming air comes in through the air duct frictional heat is produced which is the third form of undesirable heat due to incoming air and is to be removed. This friction heat is defined by Fanning friction factor expressed as follows in terms of the duct diameter, fluid density, fluid velocity, and the pressure gradient equivalent to the frictional resistance per unit length of duct.

$$f = \frac{-dP_d g_c dw}{2\bar{V}^2 dx} \qquad (30)$$

Solving the above equation for the pressure gradient yields

$$dp_d = \frac{-2f\ \bar{V}^2 dx}{g_c\ dw} \qquad (31)$$

where

dp_d = pressure gradient in lb per sq. ft.

f = friction factor, dimensionless

= density of air in lb per cu. ft.

$\bar{V}$ = velocity of air in the duct in ft per sec.

dx = length of the air duct in ft.

dw = diameter of the duct in ft.

g_c = Newton's conversion factor, 32.2 ft-lb mass per (lb. force)(sec^2)

The above units were in ft-lb system. A conversion factor of 3.2405×10^{-4} converts ft-lb to Kcal. which conformes with the units in sinesible heat and latent heat.

The velocities in the air duct and in the room were assumed to be uniform, and so their relationship is shown as below:

$$A_d \bar{V} = A_r v$$

$$\bar{V} = \frac{A_r v}{A_d}$$

A_r = cross-sectional area of the room in perpendicular to the direction of the air flow

A_d = cross-sectional area of the duct

v = air velocity in the room

The velocity in the room was about 1% of that in the air duct and so its contribution to the frictional loss was discarded. Since the main interest in this work was the application of the system analysis and optimization techniques the present design of the system was not in detail. For the same purpose the frictional losses due to fittings and values, expansion and contraction were not considered.

The density of air varies slightly with the temperature. For our purpose the average of the densities between $0^{\circ}C$ and $50^{\circ}C$ at one atmosphere was used — .0721 lb. per cu. ft.

The appropriate friction factor f to be used depends on the typed of flow defined by the Reynolds number. The Reynolds number is expressed in terms of the diameter of the duct, the velocity, density and viscosity of the fluid in the duct as follows

$$N_{Re} = \frac{D\bar{V}\rho}{u} \tag{32}$$

N_{Re} = Reynolds number, dimensionless

D = diameter of the duct

$\bar{V}$ = velocity of the fluid in the duct

ρ = density of the fluid in the duct

u = viscosity of the fluid in the duct.

If $N_{Re} < 2000$, the flow is laminar and the f to be used was [17]

$$f = \frac{16}{N_{Re}} \tag{33}$$

If $N_{Re} > 2000$, the flow is turbulent and the f to be used was [17]

$$f = .0014 + \frac{0.125}{N_{Re}^{.32}} \tag{34}$$

The frictional energy due to the frictional resistance is the energy per unit time required to overcome this resistance. This energy can be expressed in terms of the pressure gradient and the volumetric flow and being in ft.-lb. per hour was converted to Kcal. per hour to conform with that of sensible heat and latent heat by using a conversion factor. This relationship is shown below;

$$SS_3 = p_d Q \times 3.2405 \times 10^{-4} \text{ Kcal/hr.} \qquad (35)$$

Q = volumetric flow rate in cu. ft. per hour

Assumptions used in the computation of friction loss are:

(1) Air was incompressible and the air in the enclosed area was completely mixed;

(2) The density of air was taken as .0721 lb. per cu. ft.; at one atm. between $0^{\circ}C$

(3) The air in the duct was under constant pressure and temperature.

(4) The velocity of air in the duct was uniform.

(5) The friction loss of air flow in the room was considered negligible.

(6) The effects of the roughness of the duct and of heat transfer on friction factor was considered negligible.

The objective function which is the total energy is given below

$$\text{Minimize } SS = SS_1 + SS_2 + SS_3$$

$$= M_2 \times CS_2 \times \frac{(T_2 - t_a)}{1000} + M_2 \times (W_2 - W_1) \times \frac{575}{1000}$$

$$+ P_d Q \times 3.2405 \times 10^{-4} \qquad \text{Kcal./hr.} \qquad (36)$$

VI-B. Summary of Equations:

The comfort condition was defined by Fanger's comfort equation and was used as one constraint in optimization. For any combination of the inside room temperature, t_a, the partial pressure of water vapour in the roon, P_a, and the room air velocity, v, Fanger's comfort equation must be satisfied. It is shown below:

$$V = \left| \frac{A + CP_a + Dt_a + 5.95 + E[(-FP_a - Gt_a + W)^4 - (t_a + 273)^4]}{x(-YP_a - Zt_a + U)} \right|^2 \qquad (17)$$

where all the quantities are constants except t_a, P_a and v. Thus, for a given level of activity, Fanger's comfort equation is a function of t_a, P_a and v only. This relationship can be generally expressed as below.

$$\text{Comfort} = f_4 (t_a, P_a, v) \qquad (17a)$$

The other constraints were:

$$.1\text{m/sec.} < v < 2.6 \text{ m./sec.} \qquad (14)$$

$$0\% < RH < 100\% \qquad (14a)$$

The problem was to minimize the following objective function

$$SS = SS_1 + SS_2 + SS_3$$

$$= M_2 \times CS_2 \times \frac{(T_2 - t_a)}{1000} + M_2 (W_2 - W_1)\frac{575}{1000}$$

$$+ P_d Q \times 3.2405 \times 10^{-4} \quad \text{Kcal./hr.} \qquad (37)$$

Subject to the constraints of Equations (17) and (14), for a given outside condition, T_2 and P_{a2}, the objective function is a function of t_a, P_a and v only. Thus, Equation (37) can be written as

$$SS = f_5 (t_a, P_a, v)$$

On examining Equation (17) it was observed that among the three variables of t_a, P_a and v only two of them - t_a and P_a are independent. v is

a function of t_a and P_a. Thus, a series of combinations of t_a and P_a were tried. At each combination the velocity and RH constraints were checked. If the constraints were satisfied, then the corresponding objective function was computed. Three objective function values were compared at a time. The highest objective function value was then replaced by a new objective function corresponding to a new combination of t_a and P_a. The Simplex search technique was used for this optimization. This technique was described in detail in Appendix II, Part I.

IV-C. The computational procedure was summarized as follows:

1. T_a and P_a were chosen arbitrarily. With t_a the saturated vapour pressure (P_S) in the enclosed area was obtained from Equation (24). RH was then computed from Equation (24a) and checked with the RH constraint of equation (14a).
2. If RH constraint was satisfied, the same t_a and P_a values were substituted into Equation (17) to compute for v which was then checked with the velocity constraint of equation (14).
3. If the velocity constraint was satisfied, then the Simplex pattern search technique (Appendix II, Part I) was applied here. The initial values of t_a and P_a became the coordinates of the first point p_1 and the same t_a, P_a and the corresponding v values were substituted into equation (37) to obtain the objective function S_1 corresponding to p_1.
4. Similarly, points p_2 and p_3 and their corresponding objective functions of S_2 and S_3 were obtained.
5. S_1, S_2 and S_3 were compared and the point with the highest value in the objective function was replaced by a new point which was obtained by one of the following three operations: Reflection, expansion and contraction.

6. Every new point obtained was checked with the velocity and relative humidity constraints. If the constraints were satisfied, the Simplex search technique was then applied. This process was repeated until the minimum point was reached.
7. The results are shown in Table 3 and in Figures 11 through 19. The computer flow diagram for optimization is shown in Figure 20.

VI-D. Numerical Results:

Three starting points of $P_1(t_a = 33, P_a = 10)$, $P_2(t_a = 36.3, P_a = 10)$ and $P_3(t_a = 33, P_a = 13)$ were used to initiate optimization calculation for the first case in which the first outside condition of $50^{\circ}C$ and 100% RH and sedentary activity (52 Kcal./m^2h.). P_1 and P_3 were within the feasible region of the comfort equation (Figure 6). P_2 was outside the region. However, by contraction P_2 was brought within the feasible region and the search began. P_2 and P_3 were chosen in such a manner that the t_a increment in P_2 was about 10% of t_a in P_1 and the P_a increment in P_3 was about 30% of P_a in P_1. The time required to obtain the solution depended very much on the increment chosen and usually it was from 10% to 30%. It took 130 evolutions to arrive at the optimum point.

For the next activity (83 Kcal./m^2hr) and the rest of the activities at those outside conditions the search always started with the same initial points: $P_1(t_a = 33, P_a = 10)$, $P_2(t_a = 36.3, P_a = 10)$ and $P_3(t_a = 33, P_a = 13)$. The respective number of evaluations and time required for each activity at three outside conditions are shown in Table 5.

Provision was incorporated in the program to terminate the computation at 200th evaluation if the accuracy (.000001) specified was not yet met. However, on examination it was found that those solutions obtained by

TABLE 4. OPTIMUM VALUES FOR FOUR ACTIVITIES AT THREE OUTSIDE CONDITIONS

Outside Temp.°C (T_2)	Activity	Optimum Room Temp.°C (t_a)	Optimum Room Partial Pressure of Water Vapour	Optimum Sensible Heat Kcal./hr. (S_1)	Optimum Latent Heat Kcal./hr. (S_2)	Optimum Frictional Heat Kcal./hr. (S_3)	Optimum Relative Humidity (RH)	Optimum Room Air Velocity in m/sec (v)	Minimum Total Heat Kcal./hr. (S)
50	52	28.82	29.87	95.36	584.22	63.89	99.97	.1	743.46
	83	28.00	28.46	99.07	595.68	63.91	100.00	.1	758.66
	111	26.91	26.70	103.97	610.11	63.87	99.99	.1	777.96
	132	26.09	25.42	107.65	620.49	64.40	99.94	.1	792.55
40	52	28.82	29.87	51.42	243.06	63.87	99.97	.1	358.36
	83	28.00	28.47	55.20	255.63	63.91	99.97	.1	374.72
	111	26.91	26.70	60.21	273.31	63.88	100.00	.1	395.40
	132	26.09	25.43	64.01	282.61	63.87	100.00	.1	410.50
30	52	28.82	29.87	5.55	20.27	63.87	100.00	.1	89.69
	83	28.00	28.47	9.43	33.76	63.91	99.97	.1	107.07
	111	26.91	26.70	14.57	50.51	63.91	100.00	.1	128.99
	132	26.09	25.43	18.47	62.59	63.87	100.00	.1	144.93

Table 5. Evaluations and time required for each activity at three outside conditions

Temperature, T_2 (°C)	Activity (Kcal/m^2hr)	Evaluations	Time, minutes
50	52	130	.20
	83	200	.31
	111	149	.23
	132	200	.31
40	52	190	.29
	83	200	.31
	111	170	.26
	132	184	.28
30	52	200	.36
	83	200	.36
	111	200	.36
	132	200	.36

terminating the computations at 200th evaluation had an error of .00001 which was considered satisfactory. Therefore the evaluations were not extended beyond 200.

Table 4 summarizes the optimum values for the three variables t_a, P_a and v for three different outside conditions and four levels of activities inside. The three optimum values for the three forms of heat, dry, wet and friction, at each activity level are given. The optimum velocity was 0.1 meter per second, the lower end of the constraints, for all three conditions and four activities while the room air temperature t_a and the partial pressure of water vapour P_a varied for different activities at three outside conditions. On referring to the feasible regions of the comfort equation Figures 6 through 9 it can be seen easily that the optimum point was the intersection of the velocity line (.1) and the optimum relative humidity for that particular activity. Hence, if the lower limit of the velocity constraint were lowered, the optimum t_a and P_a would decrease in the same fashion. Due to the narrow velocity margin (.22 miles/hr vs 5.18 miles/hr) there was not much difference in the room air temperature for the four activities. The optimum values shown in Table 3 are plotted in Figures 11 through 19.

VII. DISCUSSION

The feasible region of Fanger's comfort equation are shown by the crossed lines in Figures 6 through 9. This region is within the following boundary

$$0.1 < v < 2.6 \tag{14}$$

$$0\% < RH < 100\% \tag{14a}$$

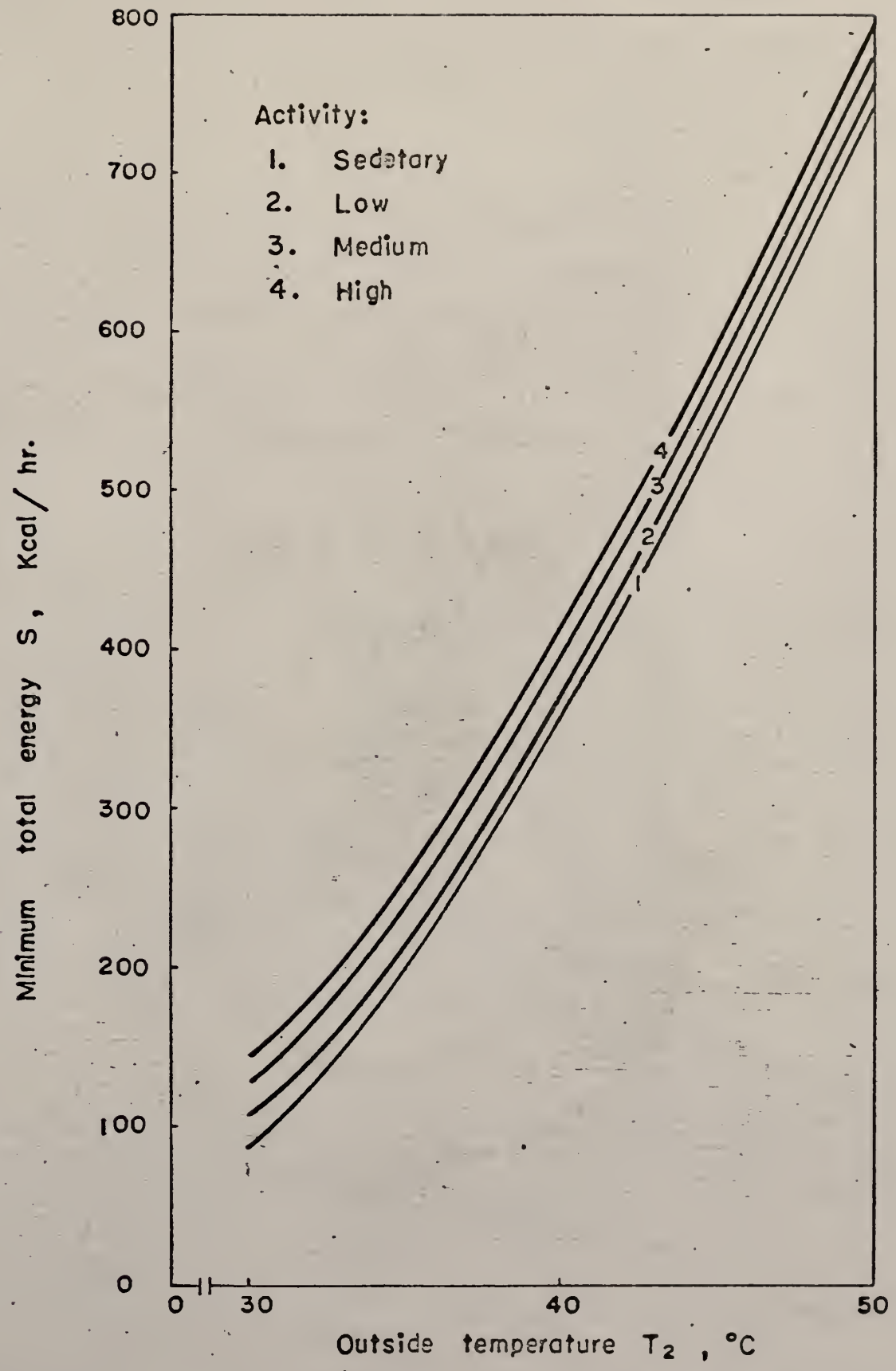

Fig.11. Effect of outside temperature on the minimum total energy for four types of activies.

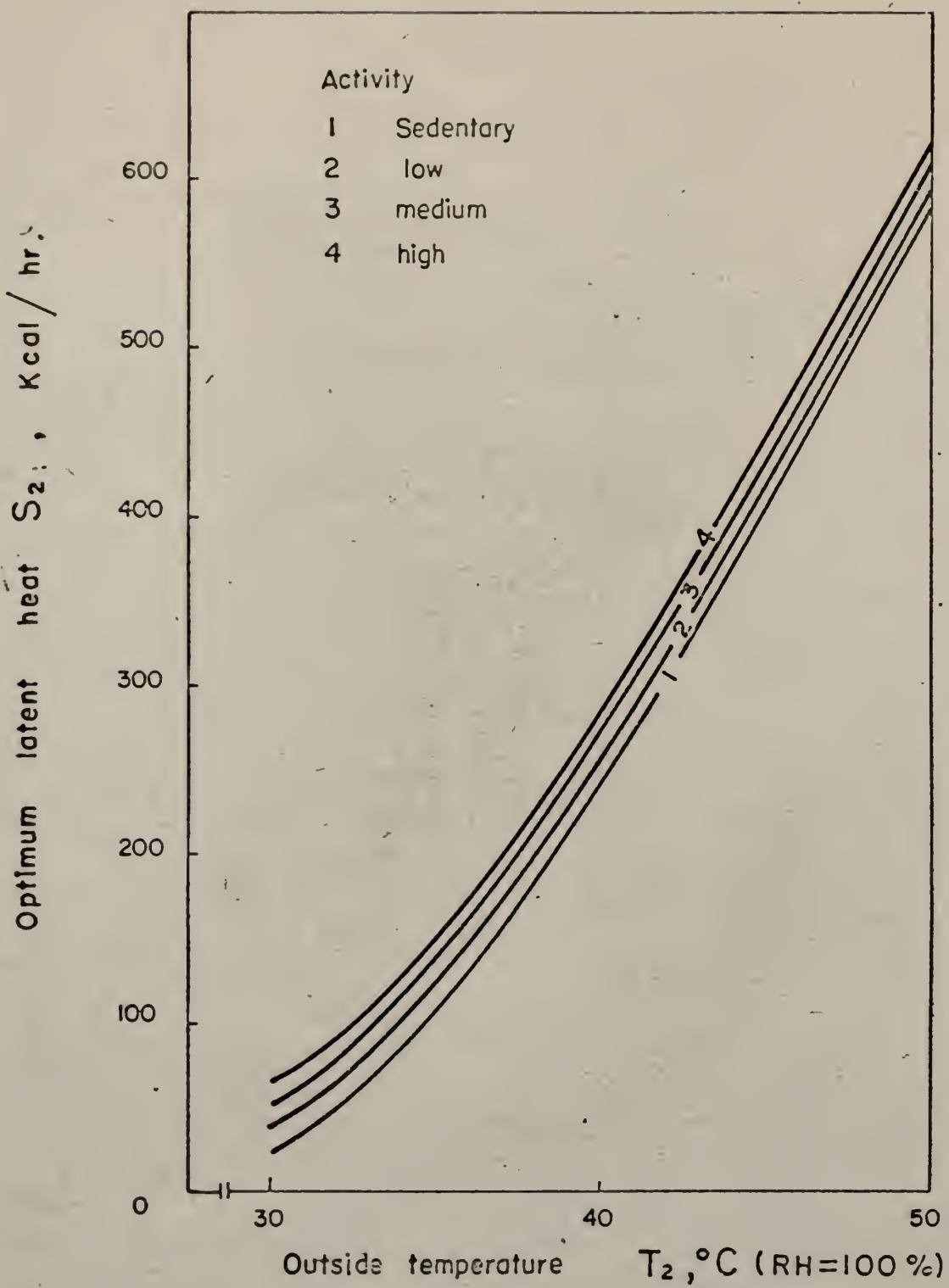

Figure 12. Effect of outside temperature on optimum latent heat for four activities.

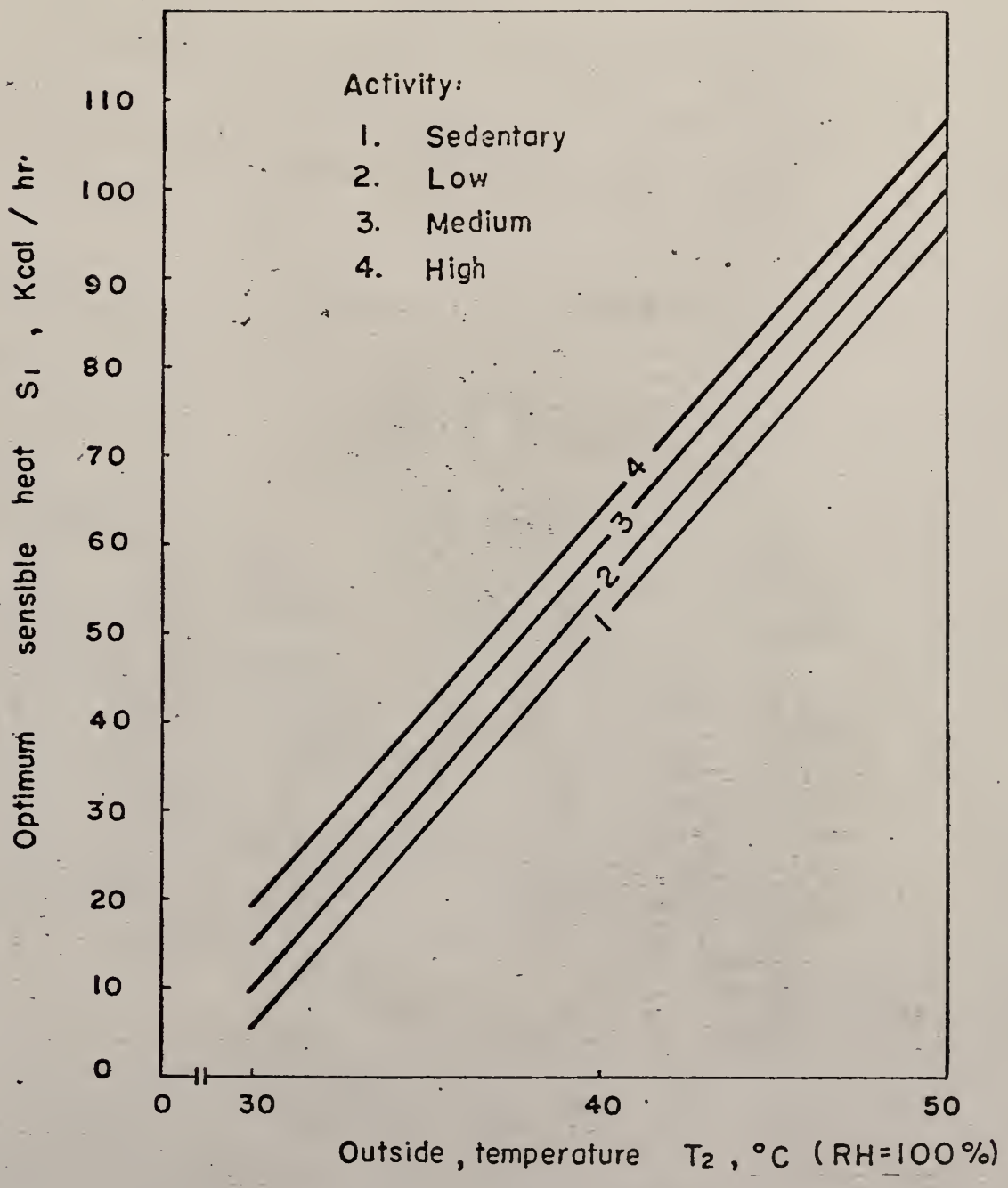

Fig. 13. Effect of outside temperature on optimum sensible heat or four activities

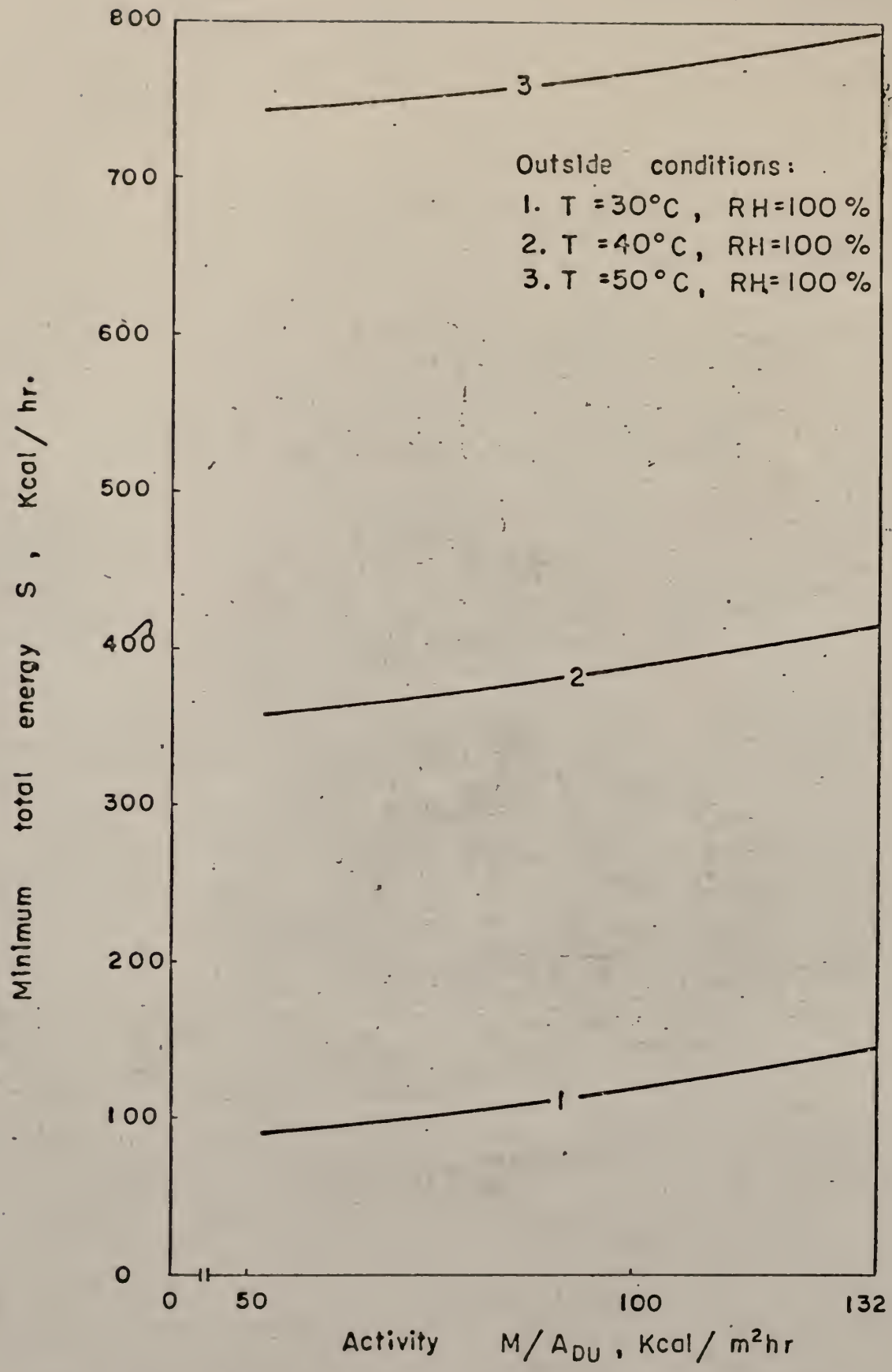

Fig. 14. Effect of activity on minimum total energy for three outside temperatures (RH=100 %)

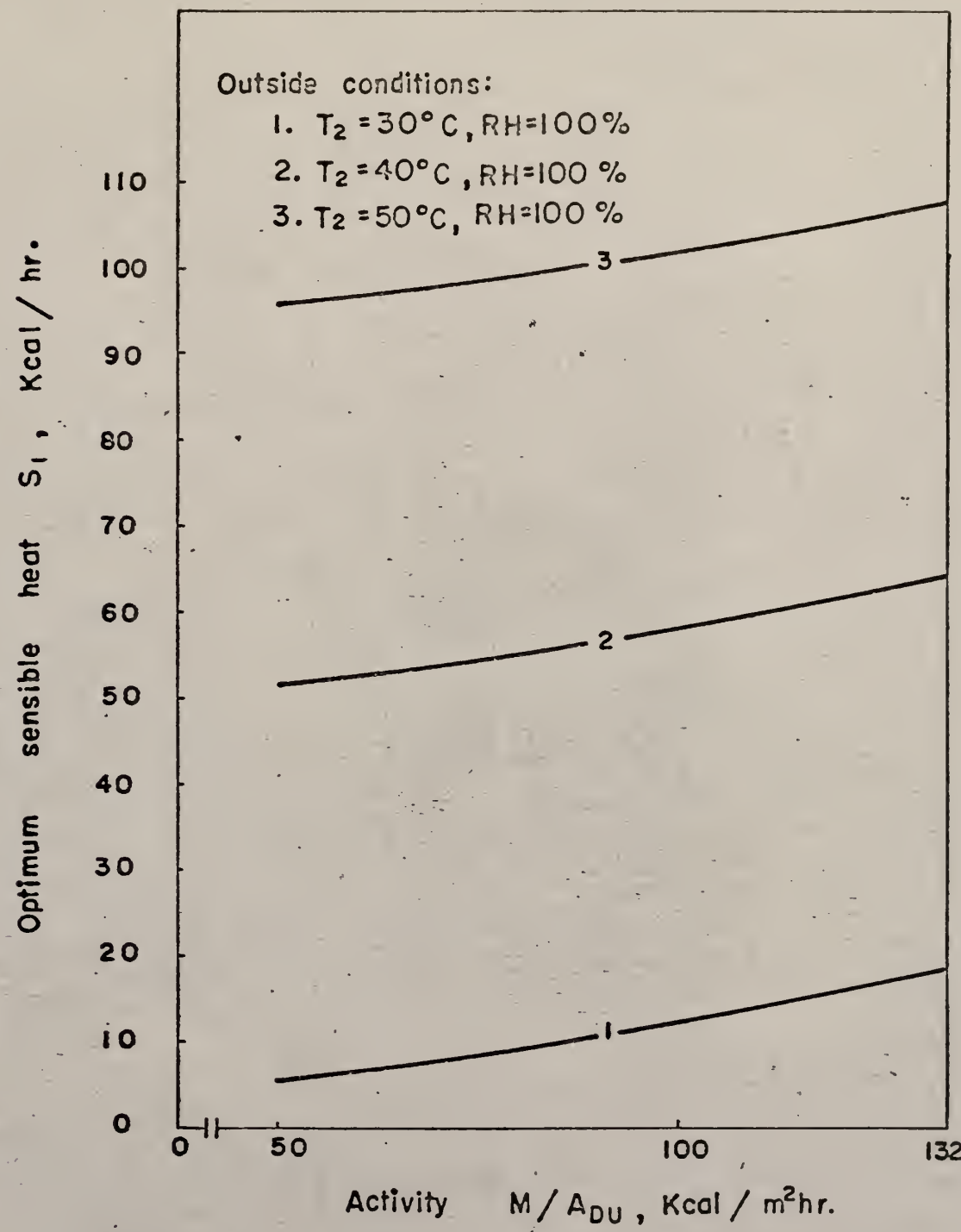

Fig. 15. Effect of activity on optimum sensible heat for three outside temperatures (RH = 100 %).

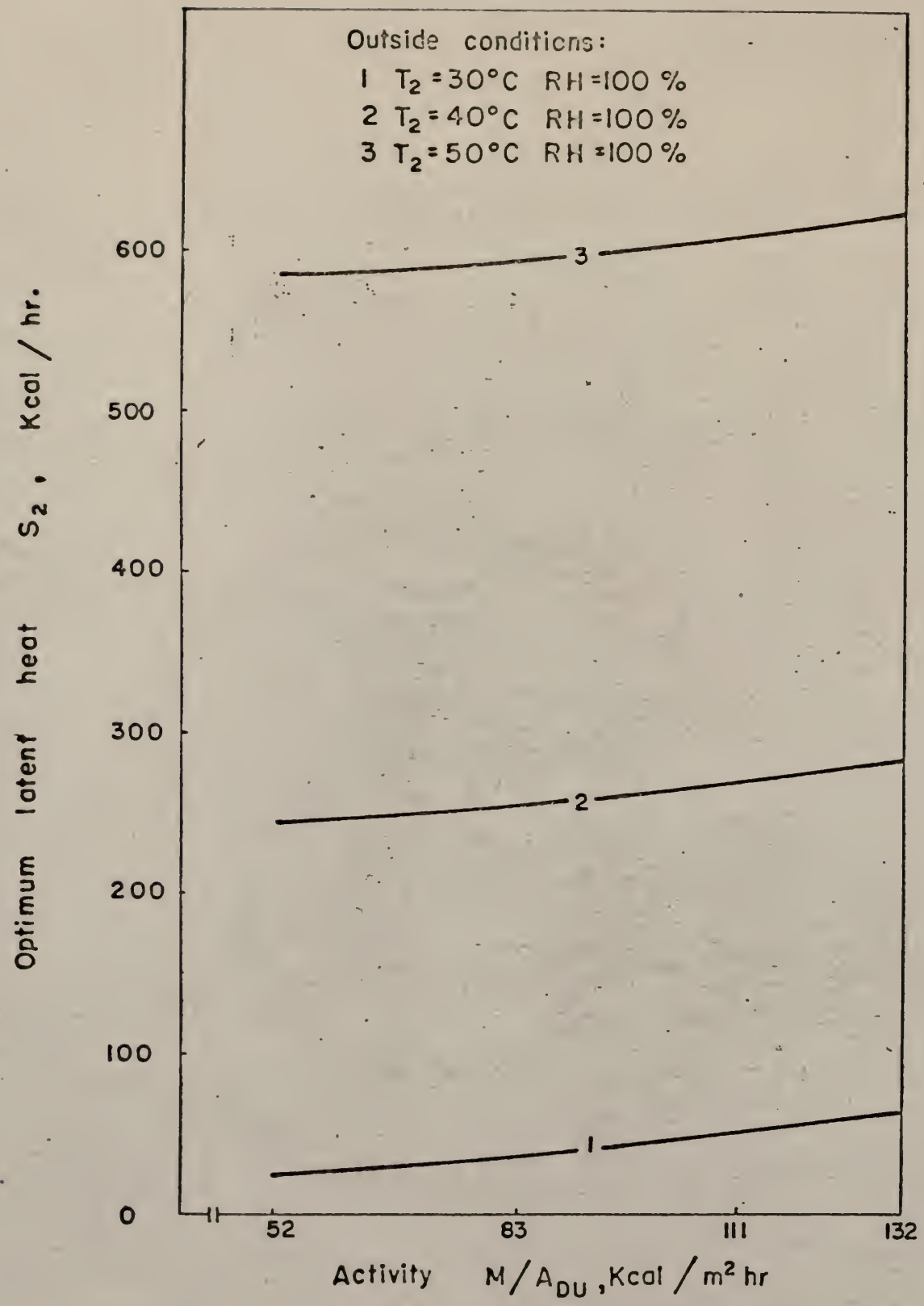

Fig. 16 Effect of activity on optimum latent heat for three outside conditions

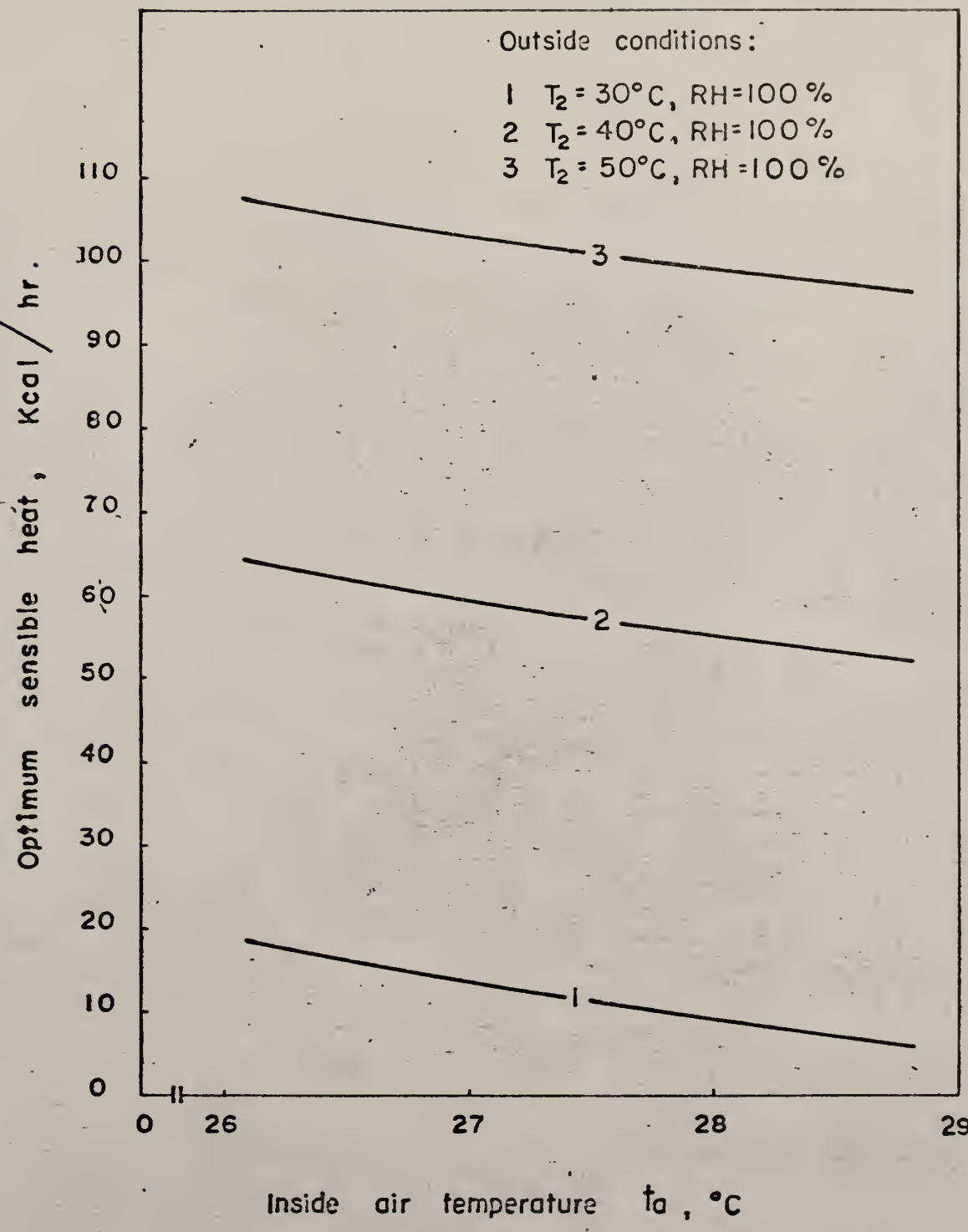

Figure 17. Effect of inside temperature on optimum sensible heat for three outside conditions and for 52-132 kc

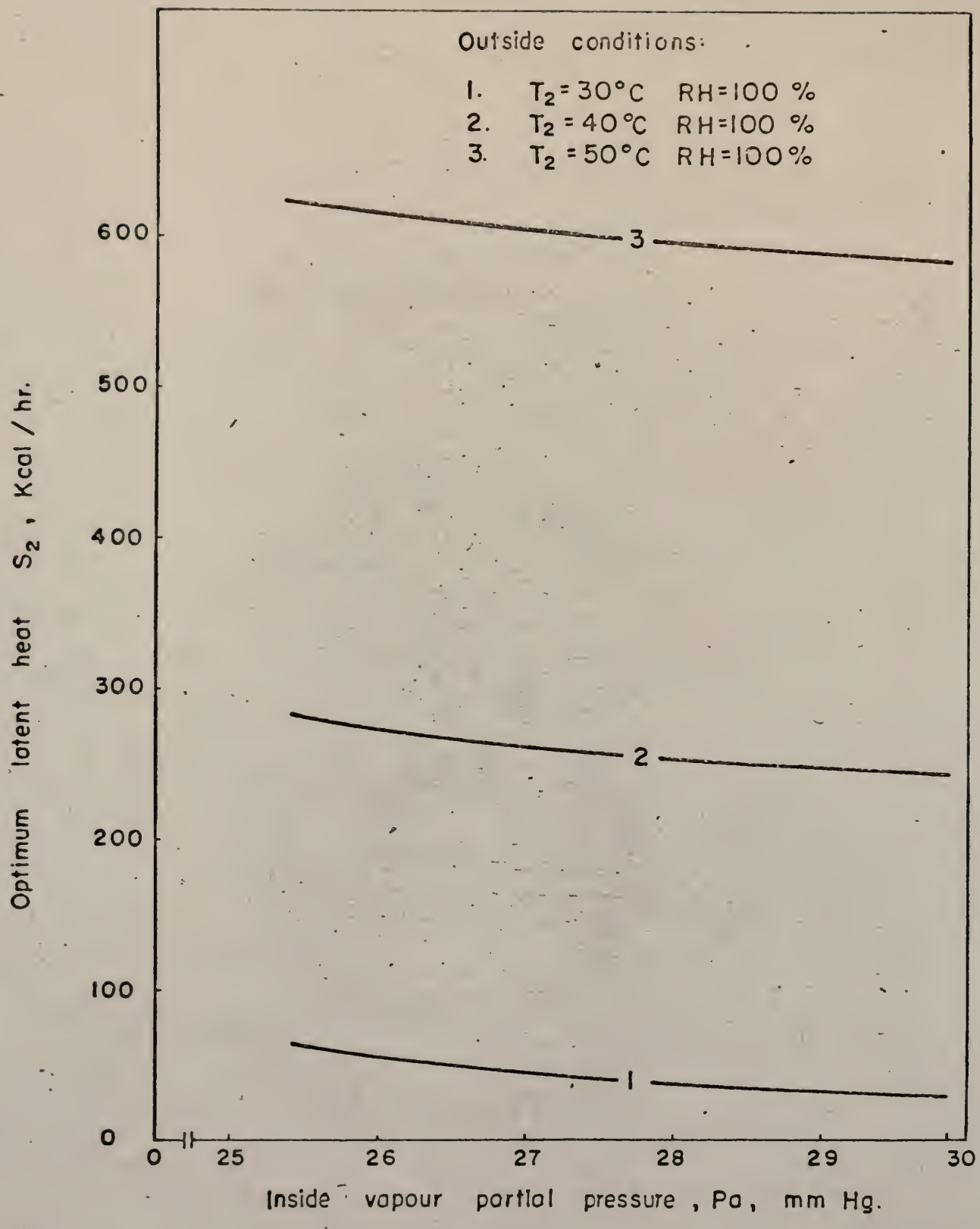

Fig. 18. Effect of inside vapour partial pressure on optimum latent heat for three outside conditions & for 52-132 Kcal/m²hr activity.

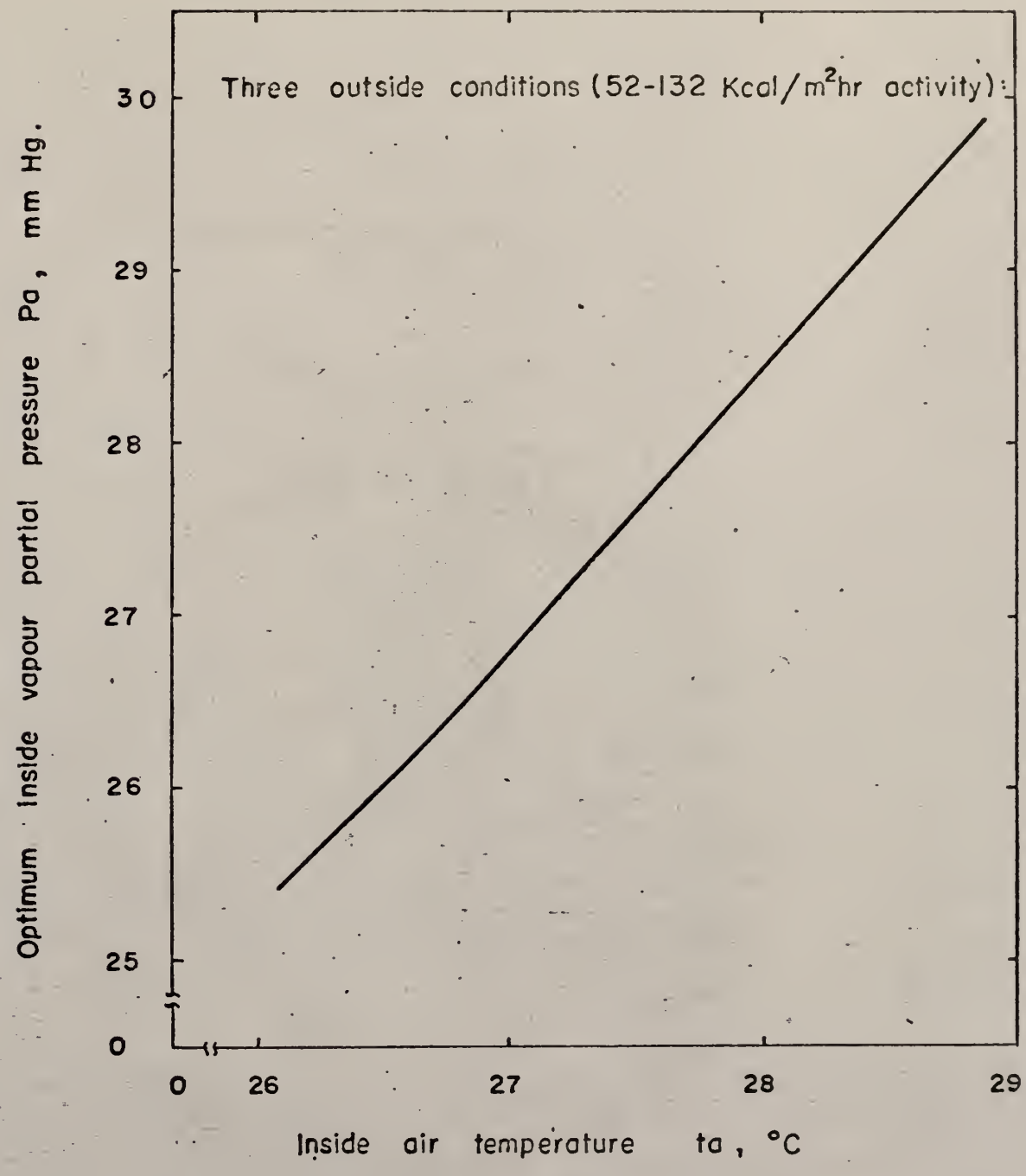

Fig. 19 · Effect of optimum inside air temperature on optimum inside vapour partial pressure for three outside conditions & for 52-132 Kcal/ m²hr activity.

where RH represented the relative humidity which is related to P_a and t_a. Again, it should be pointed out that Fanger's equation can also be used for $v < 0.1$. However, in this region free convection must be assumed and thus v will not appear in the comfort equation. The existence of the upper limit on v arises from the fact that too much draft creates uncomfortable conditions.

It should be noted that Equation (15) is a comfort equation. Under certain extreme circumstances such as in a submarine or in a spacecraft, the comfort conditions could be sacrificed for a short duration and only a survival condition might be required. In this case the feasible range of the control or independent variables t_a, P_a, and v could be enlarged considerably. The survival equation could be established and studied in essentially the same manner as the comfort equation. Furthermore, the feasible ranges of the independent variables in the comfort equation also could be enlarged under certain conditions. For example, Konz (8) showed that, with a cooling headdress, the ranges of independent variables for the comfort condition could be considerably enlarged.

The comfort equation, Equation (13) can be improved in various ways. It should be pointed out that the basic equations for comfort were Equations (5) and (6). Equation (13) was a heat balance equation based on heat transfer data and Equations (5) and (6). Not only the ranges of the parameters used in Equation (13) can be improved, heat transfer data could also be improved.

By modifying Equations (5) and (6) or by incorporating the heat accumulation term into Equation (8) or (13), dynamic comfort equations could be obtained. Such dynamic equations might be verified experimentally. The dynamic behavior of a life support system, especially in a space craft or

submarine, is a very important factor, which must be considered in its design and operation. For example, if there were a sudden disturbance (step input) in the environmental temperature, what would be the quickest (optimum) way to bring this temperature back to the normal survival temperature under the restrictions of the available equipment. Any variables other than temperature such as humidity, pressure, and undesirable chemical species in the enclosure could also be studied in essentially the same way.

Since a set of differential equations is used to represent a dynamic model, establishment of the dynamic model can be very complicated. Recently, Lee (10, 11), based on the work of Bellman, developed efficient techniques for the estimation of parameters or coefficients in nonlinear differential equations from noisy experimental data. These techniques were developed using quasilinearization and invariant imbedding.

For 50°C and 40°C with 100% RH outside conditions humidity was the major contribution to the total heat accounting for about 72% of the total heat. Next came the temperature which accounted for about 14% and the frictional heat for about 12%. However, at 30°C outside condition the frictional heat was the major contribution accounting for about 57% of the total heat; next came the latent heat accounting for about 32% while sensible heat accounting for about 9%. For all three outside conditions the sensible heat and the latent heat increased with the level of activity. The increase was more distinguished at 30°C outside condition. To the contrary frictional heat decreased with increase in the level of activity especially at 30°C outside condition. These relationships are shown in Table 6.

TABLE 6. Relationship of the three forms of heat with respect to the total heat

Outside Temp. T_2 °C	Activity M/A_{Du}	Sensible Heat Kcal./hr.	Latent Heat Kcal./hr.	Frictional Kcal./hr.	Total Head Kcal./hr.
50	52	13.10%	78.40%	8.70%	100%
	83	13.55%	78.40%	8.55%	100%
	111	13.75%	78.00%	8.31%	100%
	132	14.10%	78.00%	8.20%	100%
40	52	14.95%	66.60%	18.50%	100%
	83	15.30%	66.90%	17.60%	100%
	111	15.80%	67.10%	16.75%	100%
	132	16.00%	67.20%	16.00%	100%
30	52	6.21%	22.90%	70.90%	100%
	83	8.89%	31.50%	59.60%	100%
	111	11.40%	38.90%	49.50%	100%
	132	12.80%	42.90%	44.00%	100%

For the purpose of discussion a few other points in the feasible region of comfort equation of low activity (52 Kcal./m^2hr. in Fig. 6 beside the optimum point were taken to compute the total energy. The results are shown in Table 7. It can be seen that point was the true optimum. On perusal of equation (27) and (28) it can be seen that the higher the room temperature t_a and the partial pressure of the water vapour in the room p_a the lower are the sensible and latent heats. This leads to the fact that the optimum point should be on the upper velocity constraint — 2.6m./sec. However, on perusal of equation (35) it can be seen that the frictional heat is a function of $\bar{V}^3$. From an increase of .1m/sec. to 2.6m./sec. of the room air velocity gives an increase of 7.28 m./sec. to 189.38m./sec. for the air velocity in the duct whose cubes are 386 m^3/sec^3 and 6780000 m^3/sec^3 respectively. This in turn gives a tremendous increase in the frictional heat. From this relationship it can be seen that velocity is a major factor in this optimization problem.

TABLE 7. ENERGY AT SIX DIFFERENT POINTS IN THE FEASIBLE REGION OF COMFORT EQUATION FOR SEDENTARY ACTIVITY

POINT	ROOM AIR VELOCITY m/sec.	DUCT AIR VELOCITY m./sec.	SENSIBLE HEAT Kcal./hr.	LATENT HEAT Kcal/hr.	FRICTIONAL HEAT Kcal./hr.	TOTAL HEAT Kcal./hr.
1	.10	7.28	95.6	571	63.87	730.47
2	2.60	189.38	83.77	541.68	482286	482912
3	.10	7.28	89.17	692.18	63.87	845.22
4	2.60	189.38	78.36	668.28	482286	483033
5	.10	7.28	82.87	820.22	63.87	966.96
6	2.60	189.38	70.93	820.22	482286	483177

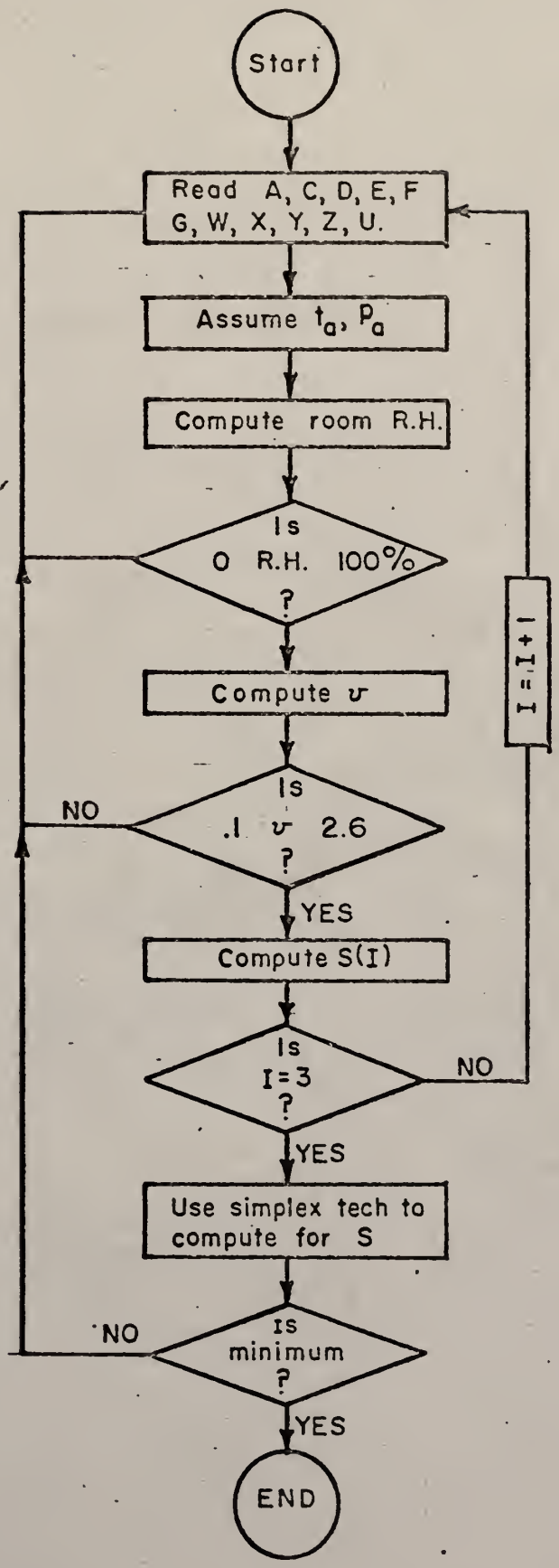

FIGURE 20. COMPUTER FLOW DIAGRAM FOR OPTIMAZATION.

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Appendix I

Newton-Raphson Method

Two methods were used in the simulation and optimization of environmental systems. Newton-Raphson method was used to solve the fourth order comfort equation in the simulation part while Simplex Search Technique was used in the optimization part. The latter was explained under "Appendix II", Part One of this work. So only Newton-Raphson method was discussed below [9]:

A Taylor series expansion around $x^{(0)}$ led to

$$f(\bar{x}) = 0 = f(x^{(0)}) + (\bar{x}-x^{(0)})f'(x^{(0)}) + \frac{(\bar{x}-x^{(0)})^2}{\alpha!} f''(x^{(0)}) + \ldots$$

$$= f(x^{(0)}) - \varepsilon^{(0)}f'(x^{(0)}) + \frac{(\varepsilon^{(0)})^2}{\alpha!} f''(x^{(0)}) + \ldots$$

with $\varepsilon^{(0)} = x^{(0)} - \bar{x}$. If the initial extimate $x^{(0)}$ was a good one, the square of the error term could be neglected. Thus,

$$f(x^{(0)}) - \varepsilon^{(0)}f'(x^{(0)}) = 0$$

$$\varepsilon^{(0)} = \frac{f(x^{(0)})}{f'(x^{(0)})}$$

It was supposed that the next improved estimate was made up as

$$x^{(1)} = x^{(0)} - \varepsilon^{(0)}$$

and also

$$x^{(1)} = x^{(0)} - \frac{f(x^{(0)})}{f'(x^{(0)})}$$

Repeating the process with $x^{(1)}$ and $\varepsilon^{(1)}$ yielded in the same way

$$\varepsilon^{(1)} = \frac{f(x^{(1)})}{f'(x^{(1)})}$$

and

$$x^{(2)} = x^{(1)} - \varepsilon^{(1)}$$

$$x^{(2)} = x^{(1)} - \frac{f(x^{(1)})}{f'(x^{(1)})}$$

In addition, $x^{(2)} = x^{(0)} - \varepsilon^{(0)} - \varepsilon^{(1)}$ which was a better estimate than $x^{(1)}$. In general terms (Newton's algorithm):

$$x^{(\gamma+1)} = x^{(\gamma)} - \varepsilon^{(\gamma)}$$

$$\varepsilon^{(\gamma)} = \frac{f(x^{(\gamma)})}{f'(x^{(\gamma)})}$$

$$x^{(\gamma+1)} = x^{(\gamma)} - \frac{f(x^{(\gamma)})}{f'(x^{(\gamma)})} \qquad \gamma = 0, 1, 2, \ldots$$

The term $- f(x^{(\gamma)})/f'(x^{(\gamma)})$ might be considered as an error term in the Newton iteration process. This error term will be minimized by a large value of $f'(x)$, thus implying that, if $f(x)$ had a strong vertical trajectory at or close to $x = \bar{x}$, convergence would be quite fast. In contrast, if $f(x)$ was nearly horizontal at $x = \bar{x}$, convergence would be

extremely slow. In the limiting case where f(x) was actually horizontal to the x axis at $x = \bar{x}$ (a maximum or minimum in the function), convergence would never occur.

The geometric significance of the Newton iteration (for real roots) was shown below

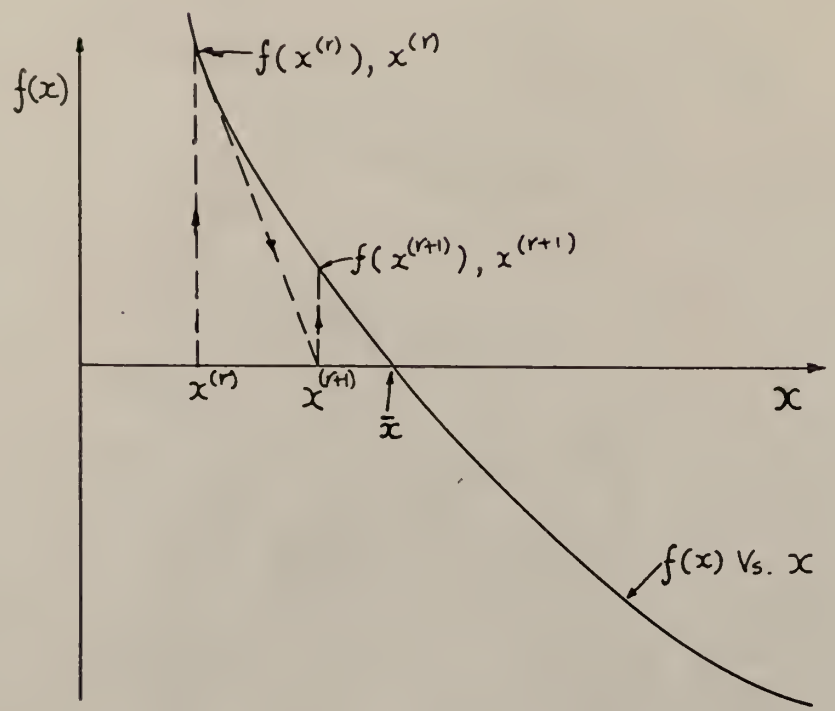

Fig. 21. Schematic diagram of Newton iteration pattern

With the estimate $x^{(\gamma)}$ for $\bar{x}$ the point $f(x^{(\gamma)}), x^{(\gamma)}$ was immediately defined on the f(x) versus x curve. If a straight line was drawn tangent to the f(x) curve at this point, the intersection on the x axis defined a new point $x^{(i)}$. Thus

$$f'(x^{(\gamma)}) = \frac{f(x^{(\gamma)})}{x^{(\gamma)} - x^{(i)}}$$

$$x^{(i)} = x^{(\gamma)} - \frac{f(x^{(\gamma)})}{f'(x^{(\gamma)})}$$

Comparison with Newton's algorithm showed that $x^{(i)} = x^{(\gamma+1)}$. Thus Newton method consisted in drawing successive tangents to f(x) curve.

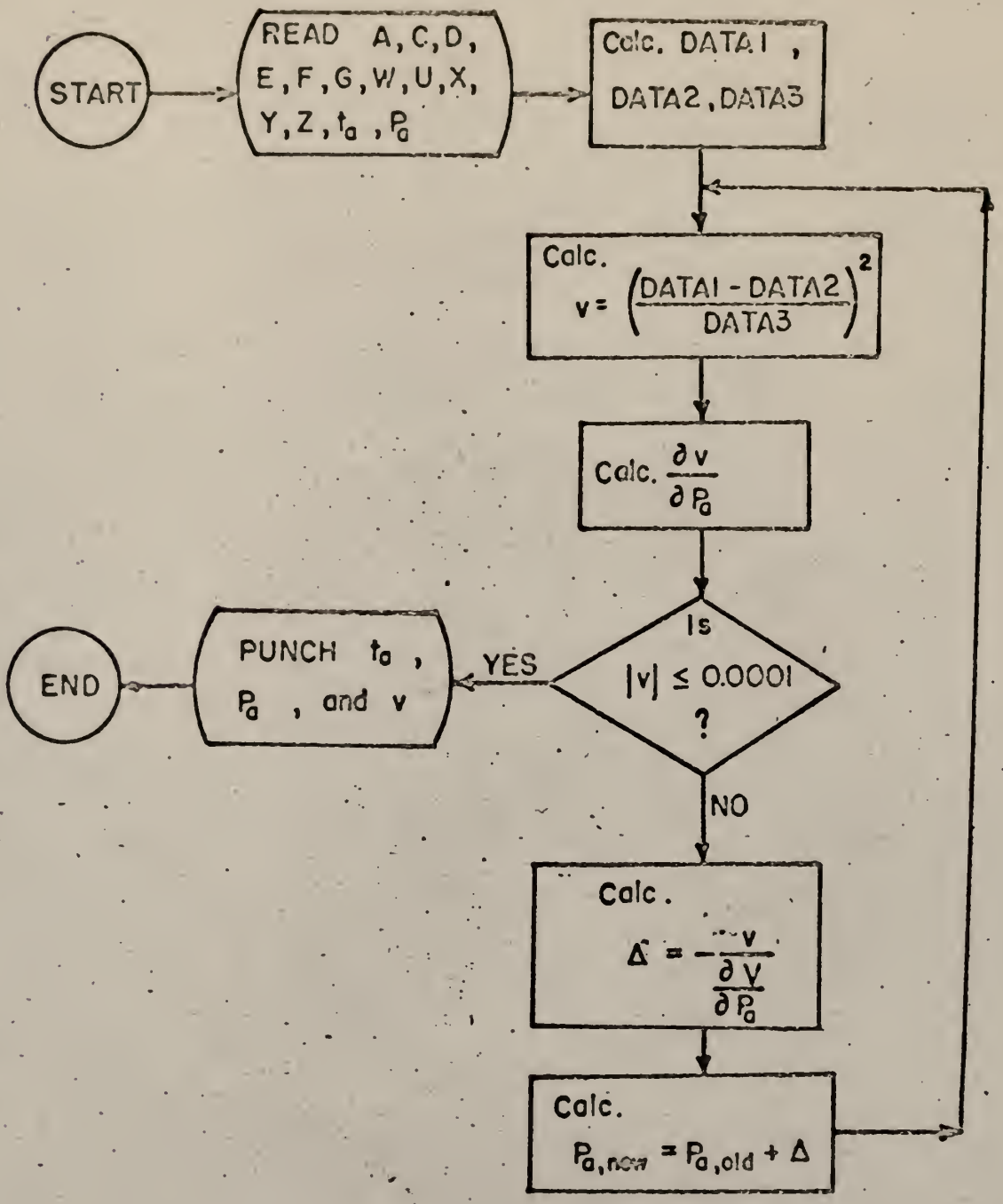

Figure 22. Computer flow diagram for the Newton-Raphson method.

Appendix II Newton-Raphson Method

```
 1 FORMAT(I3,3F15.4)
40 FORMAT(2F5.1)
   A=(389.*.4523*10.75)/(20.22*3.97)
   C=.3523
   D=.0014
   E=4.8*.00000001*1.1*.65
   F=.0380484
   G=.0002
   W=308.0574+.0117804*(389.*10.75)/(20.22*3.97)
   U=35.0574+.0117804*(389.*10.75)/(20.22*3.97)
   Y=.063414
   Z=1.00012
   X=11.44
   K=0
70 READ 40,T,P
   K=K+1
10 DATA1=A+C*P+D*T+5.95
   DATA2=E*((-F*P-G*T+W)**4-(T+273.)**4)
   DATA3=2.6*((X*(-Y*P-Z*T+U))**2)
   Q1=(DATA1-DATA2)*(DATA1-DATA2)-DATA3
   R=DATA1-DATA2
   B=(-F*P-G*T+W)**3
   Q2=(2.)*R*(C+4.*E*F*B)+5.2*X*Y*(-Y*P-Z*T+U)*X
   DELTA=-(Q1/Q2)
   S1=ABS(Q1)
   IF(S1-.01)20,20,30
30 P=P+DELTA
   GO TO 10
20 TYPE 1,K,P,T,Q1
   IF(K-5)70,50,50
50 STOP
   END
```

Appendix III Simulation of Equation (17)

```
0001          60 FORMAT(3F10.4)
0002             A=(389.*.4523*10.75)/(20.22*3.97)
0003             C=.3523
0004             D=.0014
0005             E=4.8*.00000001*1.1*.65
0006             F=.0380484
0007             G=.00012
0008             W=308.0574+.0117804*(389.*10.75)/(20.22*3.97)
0009             Z=1.00012
0010             U=35.0574+.0117804*(389.*10.75)/(20.22*3.97)
0011             X=11.44
0012             Y=.063414
0013             P=1.
0014          90 T=0.
0015          20 DATA1=A+C*P+D*T+5.95
0016             DATA2=E*((-F*P-G*T+W)**4.-(T+273.)**4.)
0017             DATA3=X*(-Y*P-Z*T+U)
0018             V=(DATA1-DATA2)*(DATA1-DATA2)/(DATA3*DATA3)
0019             WRITE(3,60)P,T,V
0020             IF(T-40.)10,50,50
0021          10 T=T+.5
0022             GO TO 20
0023          50 IF(P-60.)80,70,70
0024          80 P=P+1.
0025             GO TO 90
0026          70 STOP
0027             END
```

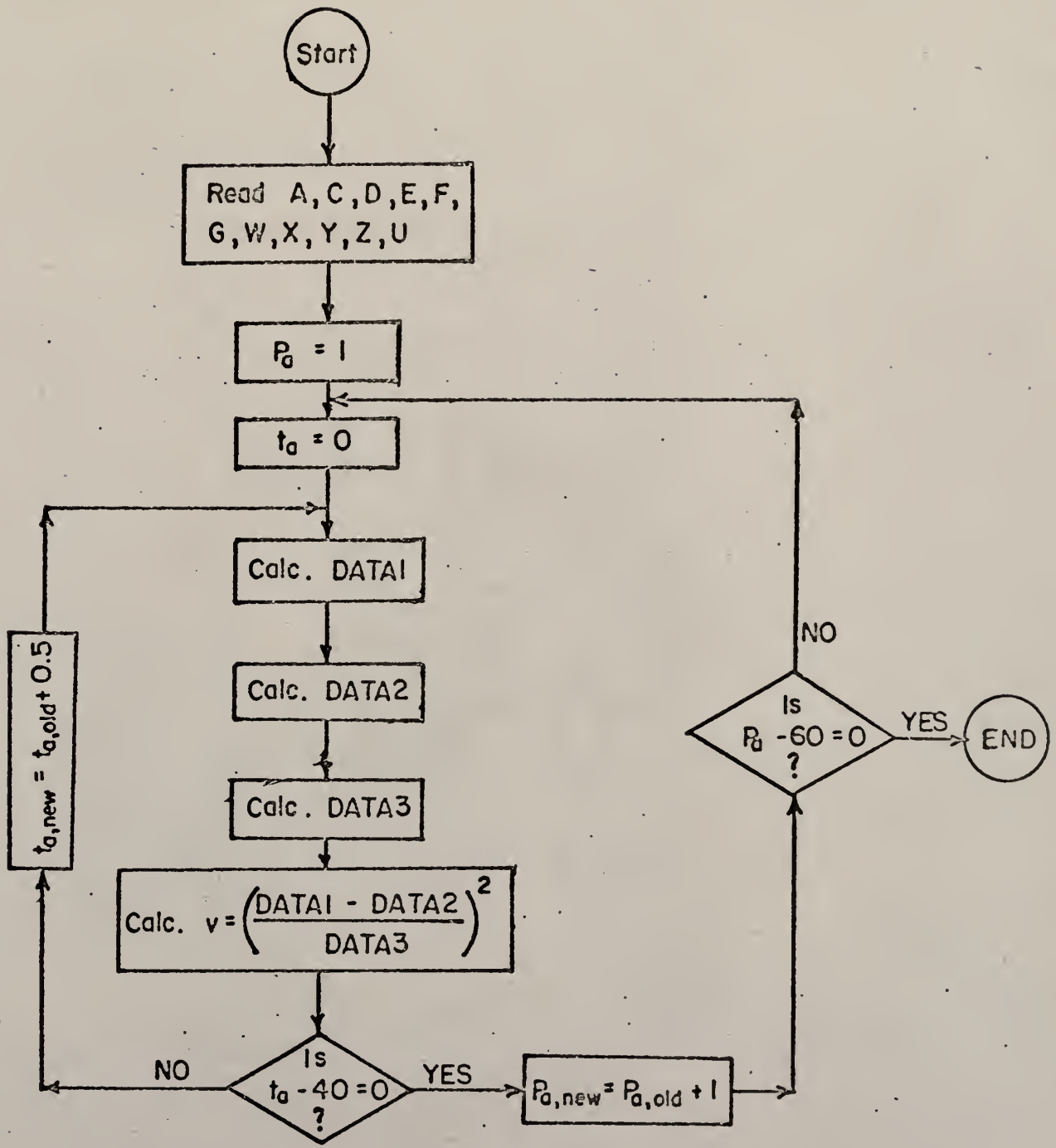

Figure 2 3. Computer flow diagram for simulation.

APPENDIX IV. COMPUTER PROGRAM FOR OPTIMIZATION

```
      DIMENSION DLTVX(27,28),S(30),DCVX(27,30)
      COMMON IX,T2
  101 FORMAT(10I5)
  102 FORMAT(7E10.4)
  103 FORMAT(/16H EVALUATION NO =I5/)
  104 FORMAT(6E13.6)
      T2=50.
      IX=1
      IY=1
      READ(1,101)NDIM,NOPT,NDIMP1,MAXNO,METHOD
      READ(1,102)ERROR,SUPLIM
      READ(1,102)((DLTVX(I,J),I=1,NDIM),J=1,NDIMP1)
  200 READ(1,102)(DCVX(I,1),I=1,NDIM)
      WRITE(3,101)NDIM,NOPT,NDIMP1,MAXNO,METHOD
      WRITE(3,104)ERROR,SUPLIM
      WRITE(3,104)(DCVX(I,1),I=1,NDIM)
      WRITE(3,104)((DLTVX(I,J),I=1,NDIM),J=1,NDIMP1)
  300 CALL GKCHEN(NDIM,METHOD,MAXNO,ERROR,SUPLIM,DLTVX,DCVX,S,KK)
      WRITE(3,104)S(NDIM+2),(DCVX(I,NDIM+2),I=1,NDIM)
      WRITE(3,104)((DCVX(I,J),I=1,NDIM),J=1,NOPT)
      WRITE(3,104)(S(I),I=1,NOPT)
      WRITE(3,103)KK
      IF(IX-4) 201,205,205
  201 IX=IX+1
      GO TO 200
  205 IF(IY-3) 206,207,207
  206 IY=IY+1
      T2=T2-10.
      IX=1
  207 STOP
      GO TO 200
      END
```

```
      SUBROUTINE GKCHEN(NDIM,METHOD,MAXNO,ERROR,SUPLIM,DLTVX,DCVX,S,KK)
      DIMENSION DLTVX(27,28),C(28),DCVX(27,30),S(30),CNTROX(27)
      COMMON IX,T2
  110 FORMAT(/19H THIS IS NEW METHOD/)
  111 FORMAT(/16H THIS IS SIMPLEX/)
  112 FORMAT(/12H THIS IS BOX/)
  113 FORMAT(/16H ****WARNING****/)
  114 FORMAT(  50H INADEQUATE GIVEN MAX. NO FOR FUNCTION EVALUATION,)
  115 FORMAT(47H INCREASING THE MAXNO OR CHANGING THE STEP SIZE/)
      GO TO (116,117,118),METHOD
  116 JMCHEN=1
      KCHEN=1
      ALPHO=1.0
      BETA=0.5
      COEFF=1.2
      GAMMA=2.0
      WRITE(3,110)
      GO TO 1
  117 JMCHEN=1
      KCHEN=2
      ALPHO=1.0
      BETA=0.5
      GAMMA=2.0
      WRITE(3,111)
      GO TO 1
  118 JMCHEN=NDIM
      ALPHO=1.3
      BETA=0.5
      WRITE(3,112)
    1 J=1
      KK=1
      CALL SUBNAM(NDIM,J,SUPLIM,S,DCVX,KK)
      K=NDIM+JMCHEN
      KLT1=K-1
      DO 3  J=2,K
      DO 2 I=1,NDIM
    2 DCVX(I,J)=DCVX(I,1)+DLTVX(I,J-1)
      CALL SUBNAM(NDIM,J,SUPLIM,S,DCVX,KK)
    3 CONTINUE
    4 M=K
      ALPHA=ALPHO
      CALL ORDER(M,NDIM,S,DCVX)
      DO 5  I=1,KLT1
    5 C(I)=1.
      CALL CNTROD(NDIM,KLT1,C,CNTROX,DCVX)
    6 DO 7  I=1,NDIM
    7 DCVX(I,K+1)=CNTROX(I)+ALPHA*(CNTROX(I)-DCVX(I,K))
      J=K+1
      CALL SUBNAM(NDIM,J,SUPLIM,S,DCVX,KK)
      IF(KK-MAXNO)8,8,36
    8 GO TO (9,9,23),METHOD
    9 IF(S(K+1)-S(1))10,10,23
   10 DO 11 I=1,NDIM
   11 DCVX(I,K+2)=CNTROX(I)+GAMMA*(DCVX(I,K+1)-CNTROX(I))
      J=K+2
      CALL SUBNAM(NDIM,J,SUPLIM,S,DCVX,KK)
```

```
      IF(KK-MAXNC)12,12,36
   12 GO TO (16,13),KCHEN
   13 IF(S(K+2)-S(1))14,14,21
   14 S(K)=S(K+2)
      DO 15 L=1,NDIM
   15 DCVX(L,K)=DCVX(L,K+2)
      GO TO 35
   16 IF(S(K+2)-S(K+1))17,17,21
   17 S(K)=S(K+2)
      DO 18 L=1,NDIM
   18 DCVX(L,K)=DCVX(L,K+2)
      M=K
      CALL ORDER(M,NDIM,S,DCVX)
      CALL SCHECK(K,SUM,NDIM,S)
      IF(SUM-ERROR)37,37,19
   19 CVALUE=2*NDIM-1
      DO 20 I=1,KLT1
      C(I)=CVALUE
   20 CVALUE=2*NDIM-2
      CALL CNTROD(NDIM,KLT1,C,CNTROX,DCVX)
      ALPHA=ALPHO*COEFF
      GO TO 6
   21 S(K)=S(K+1)
      DO 22 L=1,NDIM
   22 DCVX(L,K)=DCVX(L,K+1)
      GO TO 35
   23 IF(S(K+1)-S(K-1))21,21,24
   24 IF(S(K+1)-S(K))25,25,27
   25 S(K)=S(K+1)
      DO 26 I=1,NDIM
   26 DCVX(I,K)=DCVX(I,K+1)
   27 DO 28 I=1,NDIM
   28 DCVX(I,K+1)=CNTROX(I)+BETA*(DCVX(I,K)-CNTROX(I))
      J=K+1
      CALL SUBNAM(NDIM,J,SUPLIM,S,DCVX,KK)
      IF(KK-MAXNC)29,29,36
   29 IF(S(K+1)-S(K))30,30,32
   30 S(K)=S(K+1)
      DO 31 I=1,NDIM
   31 DCVX(I,K)=DCVX(I,K+1)
      GO TO 35
   32 DO 34 J=2,K
      DO 33 I=1,NDIM
   33 DCVX(I,J)=(DCVX(I,1)+DCVX(I,J))/2.
      CALL SUBNAM(NDIM,J,SUPLIM,S,DCVX,KK)
   34 CONTINUE
      IF(KK-MAXNC)35,35,36
   35 CALL SCHECK(K,SUM,NDIM,S)
      IF(SUM-ERROR)37,37,4
   36 WRITE(3,113)
      WRITE(3,114)
      WRITE(3,115)
      GO TO 40
   37 DO 38 I=1,KLT1
   38 C(I)=1.
      CALL CNTROD(NDIM,KLT1,C,CNTROX,DCVX)
      DO 39 I=1,NDIM
   39 DCVX(I,K+1)=CNTROX(I)
      J=K+1
```

```
      CALL SUBNAM(NDIM,J,SUPLIM,S,DCVX,KK)
   40 RETURN
      END
```

```
      SUBROUTINE SUBNAM(NDIM,J,SUPLIM,S,DCVX,KK)
      DIMENSION S(30),DCVX(27,30),X(27),XOPT(27)
      COMMON IX,T2
    1 FORMAT(31H THE OPTIMUM FUNCTION VALUE IS E13.6)
    2 FORMAT(6E13.6)
    3 FORMAT(10I4)
  104 FORMAT(6E13.6)
  999 FORMAT(9F16.2)
      IF(J-1)4,4,5
    4 KCONT=10
      ERR=10.
      GO TO 6
    5 KK=KK+1
    6 DO 7  I=1,NDIM
      X(I)=DCVX(I,J)
    7 CONTINUE
      GO TO (20,21,22,23),IX
   20 ADUM=52.
      E=4.8*.00000001*1.1*.65
      GO TO 40
   21 ADUM=83.
      E=4.8*.00000001*1.1*.75
      GO TO 40
   22 ADUM=111.
      GO TO 40
   23 ADUM=132.
   40 TK2=273.+T2
      R=62.361
      SP1=EXP(20.98-(5307.02/(273.+X(1))))
      RH=100.*X(2)/SP1
      IF(RH.LE.0.) GO TO 16
      IF(RH.GT.100.) GO TO 16
      A=.4525*ADUM
      C=.3523
      U=35.7+.019634*.6*ADUM-1.071*.6
      W=308.7+.019634*.6*ADUM-1.071*.6
      G=.00012
      F=.0380484
      D=.0014
      O=11.44
      Y=.062414
      Z=1.00012
      DATA1=A+C*X(2)+D*X(1)+5.95
      DATA2=E*(((-F*X(2)-G*X(1)+W)**4)-((X(1)+273.)**4))
      DATA3=O*(-Y*X(2)-Z*X(1)+U)
      V=((DATA1-DATA2)/DATA3)**2
      WRITE(3,104) V
      IF(V.LE..1) GO TO 16
      IF(V.GT.2.6) GO TO 16
      SP2=EXP(20.98-(5307.02/(273.+T2)))
      PA2=SP2
      W1=(18.*X(2))/(29.*(760.-X(2)))
      W2=(18.*PA2)/(29.*(760.-PA2))
      VSP2=R*TK2/(28.8*(760.-PA2))
      XM2=10.*60.*28.32/VSP2
      CS1=.238+.46*W1
```

```
      CS2=.238+.46*W2
      SEN=XM2*CS2*(T2-X(1))/1000.
      XLAT=XM2*(W2-W1)*575./1000.
      VIT=(12.*V)/(3.1416*.229*.229)
      CVIT=VIT*3.27
      RE=.458*1.293*VIT*10./(.018)
      IF(RE-2000.) 110,120,120
  110 FR=16./RE
      GO TO 150
  120 FR=.0014+.125*(RE**(-.32))
  150 PRS=2.*FR*.0721*(CVIT**2)*20./(32.2*.458)
      VOLF=3.1416*((.229*3.27)**2)*CVIT
      HF=PRS*VOLF*3600.*3.2405*(10.**(-4))
      WRITE(3,999) W1,W2,CS1,CS2,VIT,CVIT
      WRITE(3,999) RE,FR,PRS,VOLF,HF
      WRITE(3,999) SEN,XLAT,RH,T2,ADUM
      T=SEN+XLAT+HF
      S(J)=T
      IF(J-1)9,9,11
    9 DO 10 I=1,NDIM
      XOPT(I)=X(I)
   10 CONTINUE
      SOPT=T
      IF(J-1)17,17,12
   11 IF(S(1)-S(J))12,9,9
   12 IF(KK-KCONT)14,13,13
   13 WRITE(3,1)SOPT
      WRITE(3,2)(XOPT(I),I=1,NDIM)
      WRITE(3,3)KK
      KCONT=KCONT+10
   14 IF(S(J)-ERR)15,15,17
   15 WRITE(3,1)SOPT
      WRITE(3,2)(XOPT(I),I=1,NDIM)
      WRITE(3,3)KK
      ERR=ERR*0.1
      GO TO 17
   16 S(J)=SUPLIM
   17 RETURN
      END
```

```
      SUBROUTINE ORDER(M,NDIM,S,DCVX)
      DIMENSION S(30),DCVX(27,30)
      COMMON IX,T2
      K=M
      KLT1=K-1
      DO  5 I=1,KLT1
      M=M-1
      DO  4 J=1,M
      IF(S(M+1)-S(J))2,2,4
    2 A=S(M+1)
      S(M+1)=S(J)
      S(J)=A
      DO  3 L=1,NDIM
      B=DCVX(L,M+1)
      DCVX(L,M+1)=DCVX(L,J)
      DCVX(L,J)=B
    3 CONTINUE
    4 CONTINUE
    5 CONTINUE
      RETURN
      END
```

```
      SUBROUTINE CNTROD(NDIM,KLT1,C,CNTROX,DCVX)
      DIMENSION C(28),CNTROX(27),DCVX(27,30)
      COMMON IX,T2
      CSUM=0.
      DO 1  I=1,KLT1
    1 CSUM=CSUM+C(I)
      DO 3  I=1,NDIM
      AXIS=0.
      DO 2  J=1,KLT1
      CNTROX(I)=AXIS+C(J)*DCVX(I,J)
      AXIS=CNTROX(I)
    2 CONTINUE
      CNTROX(I)=CNTROX(I)/CSUM
    3 CONTINUE
      RETURN
      END
```

```
      SUBROUTINE SCHECK(K,SUM,NDIM,S)
      DIMENSION S(30)
      COMMON IX,T2
      SAVG=0.
      DO 1  L=1,K
    1 SAVG=S(L)+SAVG
      AK=K
      SAVG=SAVG/AK
      SUM=0.
      DO 2  L=1,K
    2 SUM=SUM+(S(L)-SAVG)**2
      ANDIM=NDIM
      SUM=SUM **0.5/ANDIM
      RETURN
      END
```

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IDENTIFICATION AND OPTIMIZATION OF MANAGEMENT AND ENVIRONMENTAL SYSTEMS

by

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Quezon City, Philippines, 1963

AN ABSTRACT OF A MASTER'S THESIS

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requirements for the degree

MASTER OF SCIENCE

Department of Industrial Engineering

KANSAS STATE UNIVERSITY

Manhattan, Kansas

1969

ABSTRACT

The object of this thesis was twofold: the identification of parameters in a management system and the optimization of an environmental system.

On the identification of parameters, the parameters in advertising models were recovered from (1) data without noise and (2) data with noise. Two methods, quasilinearization, and numerical integration and search were used to identify one, two and three parameters. The parameters were the contact coefficient c, the removal rate γ and the growth rate g. For quasilinearization only one parameter c was recovered. For two parameters the solution converge to different points while for three parameters the solution diverged. The numerical integration and search method recovered all the three parameters. However, in the last case of three parameters with noise in the generated data constraint had to be used before the parameters were recovered.

In the optimization of an environmental system, simulation was first performed based on Fanger's comfort equation. The parameters studied were temperature, partial pressure of water vapor and the velocity of air flow. From the simulation study the comfort zone was defined. This comfort zone was then used as the constraints in the optimization of the system. Simplex pattern search technique was used to search for the best combination of room temperature, partial pressure of water vapor and the room air velocity so that the total amount of energy removed was minimized.

For all three outside conditions of 50° C, 40° C and 30° C with 100% relative humidity the optimum room air velocity was .1 meter per second which was the lower velocity constraint. The optimum temperature was between the range of 28.83° C to 26.46° C; and the optimum partial pressure

of water vapor was 29.87 mm Hg and 20.68 mm Hg depending on the activity level of the subject. For the same activity at different outside conditions the optimum temperature and optimum partial pressure of water vapor varied very slightly because of the lower velocity and the upper relative humidity constraints which did not permit further search.