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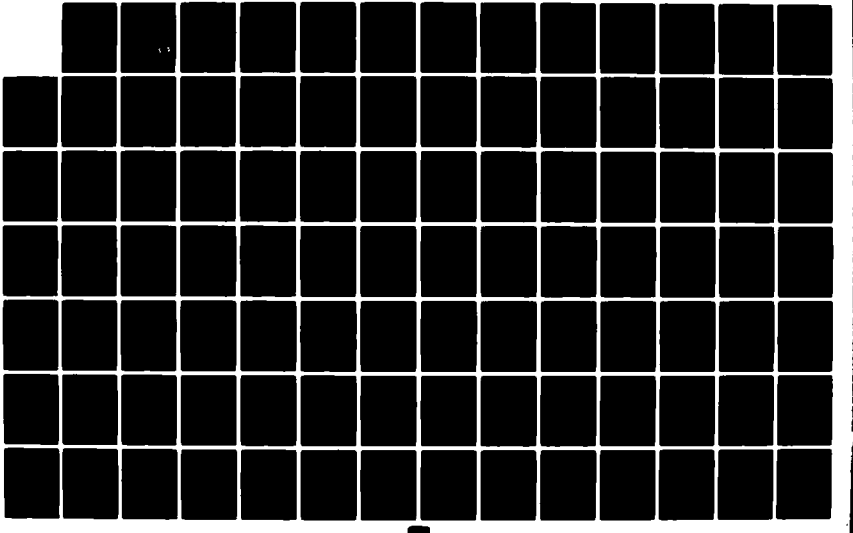

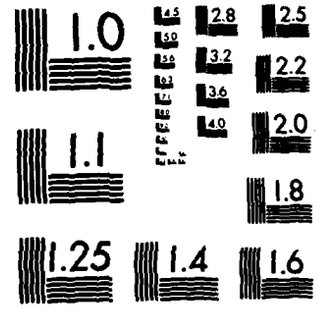

Final Report

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Nonlinear Sensitivity Analysis of Multi-Parameter Model Systems

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ABSTRACT

Large sets of coupled, nonlinear equations arise in a number of disciplines in connection with computer based models of physical, social and economic processes. Solutions for such large systems of equations must be effected by means of digital computers using appropriately designed codes. This paper addresses itself to the critically important problem of how sensitive the solutions are to variations of, or inherent uncertainties in, the parameters of the equation set. We review here, and also present further developments, of our statistical method of sensitivity analysis. The sensitivity analysis presented here is nonlinear and thus permits one to study the effects of large deviations from the nominal parameter values. In addition, since all parameters are varied simultaneously, one can explore regions of parameter space where several parameters deviate simultaneously from their nominal values.

~~We develop~~ Developed here is A theory of ~~the~~ ~~our~~ A method of sensitivity analysis, then detail the method of implementation and finally present several examples of its use to date.

I. INTRODUCTION

Sets of coupled, non-linear equations arise in a number of disciplines in connection with computer based models of physical, social and economic processes. These sets of equations may be differential, integral or algebraic. They arise in such widely different fields as reaction kinetics, combustion, air pollution, weather forecasting, upper atmosphere phenomena, seismic analysis, operations research, systems analysis, economics, etc. These model systems may contain as many as 100 equations, a very large number of parameters (in the form of coupling coefficients such as rate coefficients, transport coefficients, economic coefficients, etc.) and a very large number of output variables. Solutions for such large systems of equations must be effected by means of digital computers using appropriately designed "codes".

As is well known, the computer solution of such large sets of equations can be quite expensive. Even after such solutions have been achieved one is still faced with a critically important problem: How sensitive is the solution to variations of, or inherent uncertainties in, the parameters of the equation set? This problem of "sensitivity" is central to the understanding of the behavior of systems, and of the models representing such systems, which contain a large set of coupled equations. It is clearly important to know how sensitive the output variables are to changes of, or uncertainties in, the parameters and which of the variables are sensitive (or not sensitive) to which of the parameters. Until this information is available, any proposed model must be suspect as a valid representation of the real system. Furthermore, the accuracy to which the model parameters, i.e., coupling coefficients, need to be determined

via calculation or experiment depends upon the sensitivity of the output variables to the value of the parameters. And finally, any desired optimization of various output variables with respect to the coupling coefficients requires a knowledge of the sensitivity.

Any attempt to determine the "sensitivity" by solving the set of equations over and over again, varying one parameter at a time over a series of values while holding all the other parameters fixed at some specific values becomes prohibitive in time and expense for the large systems discussed here. This is readily demonstrated by a simple calculation. For a model system of many coupled differential equations with n parameters and m output variables, the above procedure for z different values for each of the parameters, would require z^n integrations for each of the m variables, i.e., a total of $m(z)^n$ integrations. For m, z and n large, not only will the computations be prohibitively expensive, but the printouts would be so numerous that the analysis of the results themselves will be a major problem.

In response to this need, we have developed a statistical method for the sensitivity analysis of large systems of coupled non-linear equations. The theory[1], its application to several test kinetics systems[2] and an analysis of the approximations[3] have already been presented and the reader is referred to these publications for various details which may not be covered in this paper.

The purpose of this article is to recast and further develop our method of sensitivity analysis into a form which has a number of advantages over the previous formulation[(1-3)]. This new formulation permits us to discuss sensitivity analysis from a more familiar and direct point of view. A further advantage is that the relation to more conventional sensitivity

analysis is now easily obtained. Finally, this article is user oriented. We present here all the steps required for the readers to apply this method of sensitivity analysis to their own systems.

It is very important to point out here that the implementation of our method of sensitivity analysis is very simple even though the theoretical analysis presented here appears to be quite involved. We will demonstrate this in Sections III and IV where we discuss the implementation of the method and present some specific examples.

A mathematical model of a physical system is a programmed computer algorithm which returns a prediction y (y may be a vector) for any physically realizable values of the parameters k and constants c, and over any physically meaningful range of values of the independent variables x. Such a model may return nonsense for certain combinations of values of parameters and independent variables; but we assume that the usual theory vs. experiment checks have already been carried out on the model, so that gross deficiencies are not evident.*

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*Clearly, if these conditions are not met, there is a problem at a level more basic than that which calls for a sensitivity analysis. We might mention that our experience has shown that computer algorithms frequently have been checked out only for a limited number of specific parameters values, and not over the broader range of values for which the model presumably is valid. In order to apply the sensitivity method discussed here (or any other method of sensitivity analysis), it is necessary to "tune" the algorithm to cover the broad range of values which the model is presumed to represent. In unfavorable circumstances, this may require more work than the sensitivity analysis itself.

A model typically is characterized or controlled by "parameters", as shown in figure 1. In the abstract, we might regard these parameters as being a subset of the independent variables except for a very important distinction. The true independent variables always cover a range of values (possibly infinite) during a single run of the model. The simplest example of such an independent variable is time in dynamic processes, but space and many other variables could be independent in specific problems. The parameters, on the other hand, have unique values during the course of a single "run" of the model, although it may be necessary to vary these values from one run to the next. The need for such variation may arise from any of several possible sources, several of which are indicated in Fig. 1. For example, a "physical" parameter certainly has an unique value, but this exact value may not be known because of limitations of information; only a range or distribution of values may be known. As another example, a parameter may be controllable in a particular physical circumstance only to within some range, e.g., the impedance of a variable element of an electronic circuit, or the mass loading of a spring in a mechanical system.

Separate also in definition from the independent variables and parameter are the fixed constants of the model, which do not vary within the context of the class of problems of interest to the model user, and whose values can be precisely specified. It should be noted, of course, that what is a fixed constant in the context of one situation might be a parameter in the context of another situation; the distinction depends on the particular case on hand.

The fact that the parameters can take on a range of values suggest that a statistical approach to sensitivity analysis is appropriate. Instead

of considering the effect on the output functions of one at a time variations in each of the parameters as in a "brute force" method, we will construct outputs averaged in one operation over probability distributions of all the parameters. The distribution of the parameters can arise because of experimental uncertainties or theoretical approximations, because of "ignorance" of the value within certain reasonable bounds, or might represent upper and lower limits due to "stops" on the physical controls of the systems being modeled.

Our method of sensitivity analysis proceeds by relating the probability distribution of each parameter to a frequency and one new parameter s which, as s varies, carries all the parameters through their range of variation. The parameter s is varied, and the frequencies chosen in such a way that the output variables at any fixed time become periodic in s.

The output variables can then be Fourier analyzed. As we shall show below, the Fourier coefficients represent an average of the output variables over the uncertainties of all the parameters. A unique correspondence between the Fourier coefficients for the frequency ω_ℓ and all its harmonics, and the sensitivity of the output variables to the ℓ'th parameter is established. We compress all this information into partial variances S_{ω_ℓ} which are the normalized sums of the squares of the Fourier coefficients of the fundamental frequency ω_ℓ and all its harmonics. If $S_{\omega_\ell} < S_{\omega_j}$ for a given output variable, then this output variable is less sensitive to the ℓ'th parameter than to the j'th parameter. Thus, the partial variances measure the average sensitivity of an output function to the variation (or uncertainty) of a particular parameter. This average is over the range of uncertainties of all the parameters, with their appropriate probability distributions, with the exception of the parameter being considered. For this parameter, the statistical property calculated is the variance.

The sensitivity analysis presented here is nonlinear so that it permits us to examine large deviations from the nominal parameter values. In addition, since all parameters are varied simultaneously, one explores regions of parameter space where more than one parameter is far from its nominal value. Because of this thorough and systematic exploration of the parameter space, it often turns out (see e.g. the examples of Section IV) that sensitivities of an unexpected nature are revealed. A careful study of the model will then reveal some complex coupling between variables, unexpected prior to the analysis, which leads to the observed sensitivity. In this fashion, one obtains deeper insights into the structure of the complex system being studied. Another frequent and important finding is that a number of sensitivity coefficients corresponding to a large set of parameters turn out to be negligible. This permits one to reduce the complexity of the set of model equations and focus one's attention on a greatly reduced set of equations. The applications that we present in Section IV will exhibit this feature.

The body of this paper is organized into four sections. In Section II we develop the theory of our method of sensitivity analysis. Section III details the implementation of the method and in Section IV we present several examples of its use to date. In Section V we list a number of unsolved problems on which further research would be most useful.

As previously mentioned, the implementation of the method is possible without a knowledge of the details of the analytic development. Readers primarily interested in the application of sensitivity analysis to some specific problems can by-pass Section II and go directly to Section III. The examples of Section IV will serve to show the capability and range of applicability of the method.

The analytic development of Section II is divided into several subsections which correspond to the separate steps that make up the sensitivity analysis. We first introduce the parameter uncertainties (or variations) together with a search curve procedure for exploring the values of the output function at different points in parameter space. The path of the search curve, parametized by a search variable s, is closed on itself in the parameter space so that the output function is periodic in the search variable and can be Fourier analyzed. Since the search curve is closed it cannot cover all points in parameter space. The interpretation of the Fourier coefficients as measures of sensitivity is exact only if the search curve were to cover all the parameter space. To explore this error, we introduce another space, "θ-space", which has the same dimension as the parameter space, and find that the error can be estimated and controlled. Next we note that the Fourier coefficients must be evaluated numerically as finite sums and we take into account the errors introduced by this procedure. The Fourier coefficients are then combined in a well defined prescription to yield the desired sensitivity coefficients and the precise meaning of these coefficients is detailed. This is followed by a discussion of our original procedure[1] and the relation of our nonlinear sensitivity analysis with the linear types of sensitivity analysis usually employed in the past.

II. Fourier Method of Sensitivity Analysis

A. Parameter Probability Distribution

We assume that a mathematical model of the desired physical system has been constructed. For many problems the equation set takes the form

$$\frac{d\,\underline{f}(t)}{dt} = \underline{F}(\underline{f},\underline{k}) \qquad \underline{f}(t=0) = \underline{f}_o \tag{2.1}$$

with $\underline{f}$ a vector of m output functions $(f_1, f_2, \ldots f_m)$ at time t, $\underline{k}$ a vector of n parameters $(k_1, k_2, \ldots k_n)$ which couple the nonlinear equations represented by $\underline{F}$, and with $\underline{f}(t=0) = (f_1(o), f_2(o), \ldots, f_m(o))$ a vector of given initial conditions. We assume that this set of equations can be solved numerically for $\underline{f}(t)$ for any time t once $\underline{f}_o$ and $\underline{k}$ are specified.

Now consider each of the parameters k_ℓ to range over a continuous set of values $-\infty < k_\ell < \infty$. We write

$$k_\ell = g_\ell(u_\ell) \qquad -\infty < u_\ell < +\infty\ , \quad \ell = 1, 2, \ldots, n \tag{2.2}$$

where $g_\ell(u_\ell)$ denotes some function of u_ℓ. The variable u_ℓ serves to vary the k_ℓ. In references (1-3) we chose the particular form $k_\ell = k_\ell^{(o)} \exp u_\ell$, with $k_\ell^{(o)}$ the nominal value of the parameter to permit a wide range of variation of k with u. The u_ℓ are now considered to be independent random variables with their respective probability densities $P_\ell(u_\ell)$ such that $P_\ell(u_\ell)du_\ell$ gives the probability that the random variable u_ℓ lies in the range $(u_\ell, u_\ell + du_\ell)$. Since the variables u_ℓ are not correlated, then the probability density $P(\underline{u})$ is given the product of the $P(u_\ell)$, i.e.

$$P(\underline{u}) = \prod_{\ell=1}^{n} P_\ell(u_\ell) \tag{2.3}$$

By way of example, for many problems these densities $P_\ell(u_\ell)$ will be more or less normally distributed with widths dependent on one's knowledge of the dispersion of the values of the parameters k_ℓ around the nominal value $k_\ell^{(o)}$.

We now introduce averages over these densities which, as we shall show, will lead to useful measures of sensitivity. The n dimensional $\underline{u}$-space average of a function $f(\underline{u})$ is defined as

$$\langle f(\underline{u}) \rangle \equiv \int d\underline{u}\ f(\underline{u})\ P(\underline{u}). \tag{2.4}$$

The "brute force" method of sensitivity analysis corresponds to picking a grid of points in the $\underline{u}$-space, evaluating the solution of the equation set (2.1) for the values of the parameters $\underline{k}(\underline{u})$ at these grid points and examining how the output functions change with $\underline{k}(\underline{u})$.

B. The Search Curve

In our method we construct a search curve in the $\underline{u}$-space which is a path in $\underline{u}$-space parametized by the search variable s. The search curve is constructed so that the n-dimensional $\underline{u}$-space average of the output function, Eq. (2.4) equals the one dimensional s-space average.

The translation of the probability density of the u_ℓ's into s-space is made by the introduction of n transformation functions $G_\ell(\ell=1,2,...n)$ such that

$$u_\ell = G_\ell(\sin\omega_\ell s, \tag{2.5}$$

In these equations, the ω_ℓ are a set of incommensurate frequencies, with one frequency assigned arbitrarily to each component u_ℓ of the vector $\underline{u}$. The set of equations (2.5) then is a parametric representation of an n-dimensional curve in the space of the variables $(u_1, u_2, \ldots u_n)$. Variation of s over the range $-\infty \leq s \leq +\infty$ generates a curve which traverses this n-dimensional parameter space infinitely often in each direction, but with a relative rate of traversal in each direction which is proportional to the frequency ω_ℓ assigned to that direction.

Within this broad statement, the detailed shape of the curve depends upon the specific functional forms chosen for the transformation functions G_ℓ. Inasmuch as we wish to obtain a specific distribution $P_\ell(u_\ell)$ in the ℓ-th direction, it is necessary to choose G_ℓ so that the fraction of the total arc length of the curve which lies between the values u_ℓ and $u_\ell + du_\ell$ is equal to $P_\ell(u_\ell)du_\ell$. The conditions for this equivalence were deduced by Weyl[4] and in terms appropriate for a sensitivity analysis, derived in an earlier paper in this series.[1] It was found there that if $G_\ell(x_\ell)$ is

taken to be the solution of

$$\pi(1 - x^2)^{1/2} P_\ell(G_\ell) \frac{dG_\ell(x)}{dx} = 1 \qquad (2.6)$$

with the boundary condition $G_\ell(0) = 0$, then the arc length along this curve is distributed in accordance with the previously stated requirement. This equation can be solved by quadrature for <u>any</u> distribution function P_ℓ. Thus, it is possible to construct a one-dimensional manifold which covers parameter space exactly in accordance with the requirements of the statistics.

The curve generated by the set of equations (2.5) and (2.6) can be referred to as a "search curve". As demonstrated by Weyl, the fact that the frequencies ω_ℓ are incommensurate guarantees that the curve is space-filling, by which we mean that it passes arbitrarily close to any preselected point in parameter space for which the joint distribution $\prod_{\ell=1}^{n} P_\ell(u_\ell)du_\ell$ does not vanish. Thus, the search curve is an ideal sampler of parameter space, since it seeks out, in the sense just defined, each point in the space, and it fills the space with a relative density matched to the joint distribution of the parameters.

The search curve just described is an ideal which cannot be numerically realized. It is clear that the frequencies ω_ℓ which are used in the computational analysis cannot be incommensurate. Thus, we are limited to commensurate frequencies which must be chosen to mimic as closely as possible the above requirement of a space-filling curve. We shall, in the sections that follow, discuss the errors introduced by the use of commensurate frequencies. As in our earlier work[1,2,3] we develop the theory here for <u>integer</u> frequencies. The use of such frequencies leads to a search curve that cannot fill the space but yields a <u>closed path</u> in the <u>u</u>-space. The entire traversal of the <u>u</u>-space is then accomplished by letting the search parameter s range between 0 and 2π.

C. Fourier Coefficients

The use of integer frequencies in the transformation functions, Eq. (2.5), implies that the u_ℓ's are periodic in s on the interval $(0, 2\pi)$. Since the output functions f_i are a function of s through the u_ℓ's they are, as a function of s, periodic on $(0, 2\pi)$, i.e.

$$f_i(s) = f_i(s + 2\pi). \tag{2.7}$$

The output functions can thus be Fourier analyzed to obtain their Fourier coefficients

$$\begin{aligned} A^{(i)}_{p\omega_\ell} &= \frac{1}{\pi} \int_0^{2\pi} \cos(p\omega_\ell s)\, f_i(s)\, ds; \qquad p = 0, 1, \ldots \\ B^{(i)}_{p\omega_\ell} &= \frac{1}{\pi} \int_0^{2\pi} \sin(p\omega_\ell s)\, f_i(s)\, ds; \qquad p = 1, 2, \ldots \end{aligned} \tag{2.8}$$

In terms of an average over s-space, the Eqs. (2.8) can be re-written as

$$\begin{aligned} \frac{1}{2} A^{(i)}_{p\omega_\ell} &= \langle \cos(p\omega_\ell s)\, f_i(s) \rangle \\ \frac{1}{2} B^{(i)}_{p\omega_\ell} &= \langle \sin(p\omega_\ell s)\, f_i(s) \rangle \end{aligned} \tag{2.9}$$

The importance of the Fourier coefficients in Eqs. (2.8) is that if $A^{(i)}_{p\omega_\ell}$ and $B^{(i)}_{p\omega_\ell}$ are zero for all p=1,2... then the i'th output f_i is insensitive to the values of the ℓ'th parameter k_ℓ. The Fourier coefficients of the ℓ'th fundamental and all harmonics of this ℓ'th fundamental measure the sensitivity of the output to the ℓ'th parameter. These statements will be justified in the following section.

The Fourier coefficients can be interpreted as sensitivity measures if we can show that the Fourier coefficients of a given fundamental and all

its harmonics segregate the effects of each parameter uncertainty on the output functions. That is, if the Fourier coefficients $A_{p\omega_\ell}$ and $B_{p\omega_\ell}$ (p=1,2...) are affected by the uncertainty, i.e. range of variation, in the ℓ'th parameter k_ℓ and are not affected by uncertainties in any of the other parameters, then these Fourier coefficients isolate, one by one, the uncertainties of the parameters k_ℓ on the outputs. For the integer frequencies that we use this is not strictly the case, but it is approximately true. It is only for incommensurate frequencies i.e., those for which

$$\sum_{i=1}^{n} r_i\omega_i \neq 0 \qquad -\infty < r_i < +\infty \tag{2.10}$$

with r_i integer, that the segregation of sensitivity is exact. However, we shall show that the error made in the use of integer frequencies can be quantitatively predicted and controlled. We are therefore still able to use this very useful interpretation of the Fourier coefficients as proper measures of sensitivity.

D. The $\underline{\theta}$-Space

In order to demonstrate the validity of this interpretation of the Fourier coefficients, it is necessary to visualize the search curve in an n-dimensional space which is different from the $\underline{u}$-space. Let us introduce an n-dimensional $\underline{\theta}$-space with orthogonal axes $\theta_1, \theta_2, \ldots \theta_n$ defined by

$$\theta_\ell = \omega_\ell s \pmod{2\pi}; \qquad \ell = 1, 2, \ldots n. \tag{2.11}$$

In this n-dimensional space the search curve consists of a series of parallel lines with the separation between the lines determined by the choice of integers ω_ℓ. As simple examples, consider the two different choices of integer frequencies

$$\omega_1 = 1, \omega_2 = 2 \tag{2.12a}$$

$$\omega_1 = 11, \omega_2 = 13. \tag{2.12b}$$

The two dimensional $\underline{\theta}$-space and the search curves for these frequency choices are shown in Figures 2 and 3.

It is intuitively clear that as the search curve does a better and better job of covering the $\underline{\theta}$-space, an integral of a function over s-space can equally well be carried out as a multidimensional integral over $\underline{\theta}$-space. The way to obtain a uniformly dense coverage of the $\underline{\theta}$-space is to choose ω_1 and ω_2 to be incommensurate, that is choose ω_1 and ω_2 such that

$$r_1\omega_1 + r_2\omega_2 \neq 0 \qquad -\infty < r_1, r_2 < +\infty \tag{2.13}$$

for any choices of the integers r_1 and r_2.[4] Integer frequencies cannot be incommensurate but by choosing ω_1 and ω_2 appropriately the values

of r_1 and r_2 which lead to equality in Eq. (2.13) become very large. In the two examples we have chosen, $r_1 = 2$ and $r_2 = -1$ lead to equality in Eq. (2.13) for the first choice of integer frequencies while $r_1 = 13$ and $r_2 = -11$ are required for the second choice of frequencies. Thus the latter frequency choice leads to a better coverage of the $\underline{\theta}$-space as is evident from Figures 2 and 3.

So far we have focussed on the search curve's coverage of $\underline{\theta}$-space without reference to the function which is being integrated. The accuracy of replacing the s-space average by a $\underline{\theta}$-space average not only depends on this coverage but also on the values of the integrand since we want to equate $\int f(s)P(s)ds$ with $\int f(\underline{\theta})P(\underline{\theta})d\underline{\theta}$. As an extreme example, if the function f(s) were constant as s ranged over $(0, 2\pi)$, then one could equate the s and $\underline{\theta}$-space average without error for any choice of search curve. If f(s) is a slowly varying function of s, then it will also be a slowly varying function of $\underline{\theta}$ in $\underline{\theta}$-space and the error in equating the s and $\underline{\theta}$-space integrations will be small for any choice of search curve. This error is likely to increase when f(s) and $f(\underline{\theta})$ are rapidly varying functions over the ranges of s and $\underline{\theta}$. In equating s and θ-space averages one must therefore consider both the coverage of space by the search curve and the "smoothness" property of the output function f(s).

E. Relation Between s and $\underline{\theta}$-Space Averages

Since the interpretation of the Fourier amplitudes as sensitivity coefficients will be made in $\underline{\theta}$-space it is necessary to relate quantitatively the s and $\underline{\theta}$ space averages. This relation is obtained by expressing the output function f(s) as a function of $\underline{\theta}$ and noting that, by construction, $f(\underline{\theta})$ is multiply periodic in $\underline{\theta}$ on $(0, 2\pi)$. We may thus expand $f(\underline{\theta})$ in a multiple Fourier series

$$f(\underline{\theta}) = \sum_{r_1} \sum_{r_2} \cdots \sum_{r_n} c_{r_1 r_2 \ldots r_n} \exp[-i(\theta_1 r_1 + \theta_2 r_2 + \ldots + \theta_n r_n)]$$

$$= \sum_{\underline{r}} c_{\underline{r}} \exp[-i\underline{\theta}\cdot\underline{r}] , \qquad -\infty < r_i < +\infty \tag{2.14}$$

The s-space Fourier coefficients defined in Eqs. (2.9) are a subset of all possible such coefficients, namely the subset corresponding to a fundamental frequency ω_ℓ and all its harmonics $p\omega_\ell (p=2,3,\ldots)$. In $\underline{\theta}$-space we need the corresponding Fourier coefficients for our sensitivity analysis. As discussed previously, these s and $\underline{\theta}$-space coefficients are not equal because the search curve does not, for a closed path, cover the entire $\underline{\theta}$-space. The difference between these Fourier amplitudes, i.e.

$$\frac{1}{2\pi} \int_0^{2\pi} f(s) e^{ip\omega_\ell s} ds - \left(\frac{1}{2\pi}\right)^n \int \cdots \int d\underline{\theta} f(\underline{\theta}) \exp[ip\theta_\ell]$$

is the difference between an integral calculated with the search curve, a line through $\underline{\theta}$ space, and an integral calculated over the entire $\underline{\theta}$ space. Written as averages, this difference is

$$\langle f(s)e^{ip\omega_\ell s}\rangle - \langle f(\underline{\theta})e^{ip\theta_\ell}\rangle = \varepsilon\langle f(\underline{\theta})e^{ip\theta_\ell}\rangle \tag{2.15}$$

where ε measures the relative error in equating the s and $\underline{\theta}$-space integrals. Equivalently, we can write

$$C_{p\omega_\ell} - C_{000\ldots p_\ell \ldots 000} = \varepsilon C_{000\ldots p_\ell \ldots 000} \tag{2.16}$$

where C_j is the complex Fourier coefficient defined by

$$\begin{aligned} C_j &= \frac{1}{2}(A_j - iB_j) \\ C_{-j} &= C_j^* = \frac{1}{2}(A_j + iB_j) \end{aligned} \tag{2.17}$$

and where $c_{00\ldots p_\ell \ldots 00}$ is defined in Eq. (2.14).

In reference (3) and in Appendix I of this paper we show that by appropriate choices of frequencies ω_ℓ, this error can be made as small as desired. Qualitatively, as the frequencies become more incommensurate the coverage of the $\underline{\theta}$-space (and u-space) by the search curve improves and the error made in equating s and $\underline{\theta}$-space averages decreases. This can be quantified through the introduction of an index M which is the <u>order of interference</u>. Interferences arise when frequencies in the original set $\underline{\omega}$ can combine to form another frequency of the set. Thus, if we have three parameters with associated frequencies ω_1, ω_2 and ω_3 and if, for instance, $\omega_1 + \omega_2 = \omega_3$, an interference has occurred. As M increases the interferences are postponed to higher and higher harmonics and the error decreases.

Assuming that ε is negligible by appropriate choice of the set $\underline{\omega}$, we then obtain

$$C_{p\omega_\ell} = c_{000\ldots p_\ell \ldots 000} \equiv c_{p_\ell} \tag{2.18}$$

as the desired equality of s and $\underline{\theta}$-space averages. The Fourier coefficient $c_{000\ldots p_\ell \ldots 000}$ reflects the sensitivity of the output function to the uncertainty of the ℓ'th parameter (and only to the ℓ'th parameter) since $r_i = 0$ for all $i \neq \ell$ in the $\underline{\theta}$-space Fourier coefficient $c_{r_1 r_2 \ldots r_n}$. If <u>all</u> the Fourier coefficients $c_{00\ldots p_\ell \ldots 000}$ are zero for $p_\ell = 1,2,\ldots,$ then we can conclude that the output function is not sensitive to the parameter k_ℓ. Since, by (2.18), the $\underline{\theta}$-space Fourier coefficients c_{p_ℓ} equal the s-space coefficients $C_{p\omega_\ell}$, we conclude that $C_{p\omega_\ell}$ is an appropriate measure of the sensitivity of the output to the ℓ'th parameter.

The conclusion that the Fourier coefficients $C_{p\omega_\ell}$ measure just the sensitivity to k_ℓ, can also be verified via an s-space analysis. The output as a function of s, f(s), is constructed by expressing each parameter u_i as a periodic function of s with frequency ω_i (i=1,2,...n) as in Eq. (2.5). Thus, f(s) consists of a sum of terms which oscillate at all possible linear combinations of the n frequencies $\underline{\omega}$. If we single out the frequency $p\omega_\ell$ via the Fourier coefficient $C_{p\omega_\ell}$, and if the frequencies are incommensurate, no linear combination of the other frequencies can add up to form $C_{p\omega_\ell}$ and interfere with the effect on the output from the ℓ'th parameter k_ℓ. Since we do use integer frequencies, it is necessary to introduce the concept of order of interference M as defined in Eq. (A1.4). Thus, as long as we restrict our attention to Fourier coefficients $C_{p\omega_\ell}$ for which there are no interferences, or for which the interferences have been "postponed", the sensitivity is due entirely to the uncertainty in k_ℓ.

F. Finite Fourier Coefficients

In performing the Fourier analysis on the computer, the s-space integration must be approximated by a finite summation. This procedure introduces a further error into the method, which must be analyzed. It is important to minimize this error as efficiently as that due to interferences. The finite sums are obtained by taking points from the search curve in $\underline{\theta}$-space. If we use a large number N of points for the summation we will obtain an excellent approximation to the s-space integral. However, if the order of interference M is low, the accuracy of the interpretation of the s-space average as a sensitivity measure is not good. For example, if we fix N at 100, in the 2-dimensional examples discussed in section C above, the first search curve leads to the set of points shown in Figure 2 while the second search curve leads to the set of points shown in Figure 3. Even though the first search curve is better approximated by the 100 points quadrature than the second one (since the density of points is higher for the first curve), the overall distribution of points in the second case is far more uniform. We therefore would obtain a more accurate sensitivity measure in the second case than in the first.

The error introduced via the use of finite sums for the s-space integrations can be analyzed in much the same fashion as the interference problem. We denote the numerical approximation to the exact Fourier coefficient $C_{p\omega_\ell}$ by $C^*_{p\omega_\ell}$ where

$$C^*_{p\omega_\ell} = \frac{1}{N} \sum_{q=1}^{N} f(s_q)\exp[ip\omega_\ell s_q] \tag{2.19}$$

with

$$s_q = \frac{2\pi q}{N} \qquad q = 1,2,\ldots N. \tag{2.20}$$

Here N is the number of points used in the quadrature formula and s_q ($q = 1,2,\ldots N$) labels the individual points which are chosen to be equally spaced along the search curve.‡ Following the procedure used in Eq. (2.15), we now form the difference between the s-space quadrature $C^*_{p\omega_\ell}$ and the $\underline{\theta}$-space average C_{p_ℓ} to obtain

$$C^*_{p\omega_\ell} - C_{p_\ell} = \epsilon^* C_{p_\ell} \tag{2.21}$$

where, see Eq. (2.18), $C_{p_\ell} \equiv C_{000\ldots p_\ell \ldots 000}$.

The coefficient ϵ^* in Eq. (2.21) is a measure of the error introduced by approximating the $\underline{\theta}$-space integration as a finite sum at selected points in s-space. These errors are in addition to those arising from interferences. The evaluation of ϵ^*, as a function of $\underline{\omega}$, N and the output function, is presented in Appendix II.

It is important to have a ready estimate of the error term when doing sensitivity analysis without becoming involved in long calculations for each particular case under investigation. In response to this need we have in ref. (3) developed bounds on the error which depend on $\underline{\omega}$, N, and the type of output functions being investigated. We present the salient ideas of this method in Appendix III.

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‡ The equal spacing is not necessary; however, the analysis and control of the error is facilitated by this choice. The use of other spacings may actually lessen the error. See e.g. V.I. Krylov and L.G. Kruglikova, Handbook of Numerical Harmonic Analysis, Israel Program for Scientific Translations, LTD. Jerusalem, 1969.

G. Partial Variances

The Fourier coefficients with which we have been concerned so far correspond to the fundamental and harmonics of each frequency ω_ℓ. They measure the sensitivity of an output to the variations in all the parameters such that if there is a sensitivity to the ℓ'th parameter it will show up only in the Fourier coefficients $C_{p\omega_\ell}$ (p=1,2,...). The uncertainty in the other parameters is accounted for by averaging over their respective distributions. It is apparent that other Fourier coefficients contain additional information such as for instance the joint sensitivity to parameters k_ℓ and k_j. From this point of view, we can consider the variation of the output arising from the uncertainties in all the parameters k_i, i=1, 2, ..., n and their couplings to be characterized by the variance of the output function

$$\sigma^2 = \langle f^2 \rangle - \langle f \rangle^2 \ . \tag{2.22}$$

The interpretation of this variance can be explored by expressing it in terms of the s-space Fourier coefficients C_j (and the cos and sin coefficients A_j and B_j) by using the Fourier series expansion of f(s) in Eq. (2.22). This yields

$$\sigma^2 = \sum_{j=-\infty}^{+\infty}{}' c_j^2 = \frac{1}{2} \sum_{j=1}^{\infty} (A_j^2 + B_j^2) \ . \tag{2.23}$$

where the prime on the sum excludes the j=0 term. We recognize Eq. (2.23) as Parseval's Theorem of Fourier analysis. However, we are calculating finite sums for the numerical Fourier coefficients $C_j^*(A_j^*,B_j^*)$ and must therefore modify Parseval's Theorem to obtain the numerical variance σ^{2*}. This is just

$$\sigma^{2*} = \sum_{j=-(N/2-1)}^{N/2} C_j^{*2} = \frac{1}{2}\sum_{j=1}^{N/2}(A_j^{*2} + B_j^{*2}) + \frac{1}{4}A_{N/2}^{*2} \qquad (2.24)$$

The variance σ^{2*} is thus seen to be the sum of the squares of the Fourier coefficients of all integer frequencies which enter into an N point quadrature formula.

We now construct the part of σ^2 that corresponds to the variance of the output arising from the ℓ'th parameter uncertainty when the output is averaged over the uncertainties in all other parameters. To do this, we first integrate $f(\underline{k})$ and $f^2(\underline{k})$ over all uncertainties in the parameters with the exception of the ℓ'th parameter. We then calculate the variance σ_ℓ for these partially integrated output functions using equations (2.22) and (2.23). The details of this calculation will be found in Appendix IV. This result is then modified to yield the numerical variance σ_ℓ^{2*} corresponding to the finite sums of Eq. (2.24). The ratio of this variance σ_ℓ^{2*} to the total variance σ^{2*} of Eq. (2.24) is denoted by $S_{\omega_\ell}^*$ and is the partial variance, i.e.

$$S_{\omega_\ell}^* \equiv \frac{\sigma_\ell^{2*}}{\sigma^{2*}} = \frac{\sum_{p=-(N/2-1)}^{N/2} \left|C_{p\omega_\ell}^*\right|^2}{\sum_{j=-(N/2-1)}^{N/2} \left|C_j^*\right|^2} \qquad (2.25)$$

The partial variance $S_{\omega_\ell}^*$ is the fraction of the variance of the output function due to the uncertainty in the parameter k_ℓ when the output function is averaged over the uncertainties, and coupling of uncertainties of all the other parameters k_i, $i \neq \ell$.

The partial variance can thus serve as an excellent measure of the sensitivity of the output to the uncertainty of the ℓ'th parameter. It can be used to compare quantitatively sensitivities due to uncertainties in the

different parameters k_i, i=1,2,...n, since all variances are computed relative to the total variance σ^{2*}. Clearly, the smaller the partial variance, the less the effect of the changes of k_ℓ on the output function. We can therefore order the $S^*_{\omega_\ell}$'s as a function of ℓ to obtain an ordered list of sensitivities for a given output function and between different output functions.

The partial variances $S^*_{\omega_\ell}$ will have the above interpretation only if the interferences and aliasing difficulties (see Appendix II) are minimized by proper choice of $\underline{\omega}$, and N. Since $S^*_{\omega_\ell}$ involves Fourier coefficients of high index, the appropriate values of $\underline{\omega}$, and N for the minimization of these errors unfortunately involve prohibitively large numbers of function evaluations. However, as discussed previously, the Fourier coefficients decrease in amplitude as their index increases. As a practical, computational matter, our experience has shown that only a few harmonics of a fundamental need be calculated before the amplitude becomes negligible. Thus, the relative errors in comparing the partial variances $S^*_{\omega_\ell}$ for different parameters k_ℓ are small even when only the Fourier amplitudes of the fundamental and the first few harmonics are utilized.

Let us return briefly to the unstarred, i.e. analytic values of the variance σ^2 (Eq. 2.23) and the corresponding partial variances S_{ω_ℓ} given by

$$S_{\omega_\ell} \equiv \frac{\sigma_\ell^2}{\sigma^2} = \frac{\sum_{p=-\infty}^{\infty}{}' C^2_{p\omega_\ell}}{\sum_{j=-\infty}^{\infty}{}' C_j^2} \qquad (2.26)$$

where the prime on the sums excludes the p=0, j=0 terms. Note that σ_ℓ^2 in the numerator involves only the sum of the squares of the Fourier coefficients of the fundamental and all harmonics of the ℓ'th frequency ω_ℓ while the variances σ^2 in the denominator is constructed as the sum of squares of the

Fourier coefficients of all the integer frequencies. It is readily apparent from Eq. (2.26) and the development below why the sum $\sum_{\ell=1}^{n} S_{\omega_\ell}$ of the partial variances will not equal unity. Writing the variance σ^2 in terms of the $\underline{\omega}$-space Fourier coefficients according to Parseval's theorem yields

$$\sigma^2 = \sum_{p_1}^{\infty}{}' \sum_{p_2}^{\infty}{}' \cdots \sum_{p_n}^{\infty}{}' |c(p_1,p_2,\ldots,p_n)|^2 \tag{2.27}$$

where the prime indicates that the term with all p_i's equal to zero is omitted. It is suggestive to rearrange the sum in Eq. (2.27) into groups of terms where successively larger subgroups of the coefficients $p_1,p_2,\ldots,p_n$ are nonzero. We define

$$\sigma^2_{\ell} = \sum_{p_\ell=1}^{\infty} |c(o,\ldots,p_\ell,\ldots,o)|^2 \tag{2.28a}$$

$$\sigma^2_{\ell j} = \sum_{p_\ell=1}^{\infty} \sum_{p_j=1}^{\infty} |c(o,\ldots,p_\ell,\ldots,p_j,\ldots,o)|^2 \tag{2.28b}$$

$$\sigma^2_{\ell jk} = \sum_{p_\ell=1}^{\infty} \sum_{p_j=1}^{\infty} \sum_{p_k=1}^{\infty} |c(o,\ldots,p_\ell,\ldots,p_j,\ldots,p_k,\ldots o)|^2 \tag{2.28c}$$

etc.

so that

$$\sigma^2 = \sum_{\ell=1}^{n} \sigma^2_{\ell} + \sum_{\ell=1}^{n} \sum_{j=1}^{n-1} \sigma^2_{\ell j} + \sum_{\ell=1}^{n} \sum_{j=1}^{n-1} \sum_{k=1}^{n-2} \sigma^2_{\ell jk} + \ldots \quad . \tag{2.29}$$

is written as a sum of terms with successively more complex contributions to the total variance σ^2.

We have shown above that the first term of the decomposition (2.29) corresponds to the part of total variance arising from the ℓ'th parameter uncertainty when the output is averaged over the uncertainties in all other

rate coefficients. By the same methods one can also construct $\sigma^2_{\ell j}$ by integrating $f(\underline{k})$ over all but the two parameters k_ℓ and k_j to obtain $f(k_\ell, k_j)$ and then forming the variance $\sigma^2_{\ell j}$ of this function via Eq. (2.22). One can proceed in an analogous fashion to generate the other, more complex, variances in Eq. (2.29). These higher partial variances are thus seen to contain increasingly more detailed information about the coupling of sensitivity among larger and larger groups of parameter uncertainties.

In our own investigations to date we have not exploited these higher partial variances to obtain more detailed information about the sensitivity of our test systems but we hope to explore their properties in some subsequent studies.

H. Fundamental Fourier Coefficients

In the original formulation of sensitivity analysis, references (1) through (3), our efforts centered on the Fourier sine coefficients of the fundamental frequencies, the B_{ω_ℓ} in our present notation. As shown there, these Fourier coefficients can be expressed as $\underline{u}$-space averages:

$$B_{\omega_\ell} = \frac{2}{a_\ell} \left\langle \frac{\partial f}{\partial u_\ell} \right\rangle \tag{2.30}$$

where the average was taken over the $\underline{u}$-space probability density

$$P(\underline{u}) = \prod_{j=1}^{n} a_j/\cosh(a_j u_j) \tag{2.31}$$

with the $\underline{P}(u_j,a_j)$ being bell shaped distributions whose widths are determined by the parameter a_j. We have in these papers also explored various other probability densities.

The Fourier coefficients B_{ω_ℓ} are thus seen to be directly related to the rate of change of the output function with respect to the ℓ'th parameter, averaged over the uncertainty in all the parameters. This appealing interpretation of the fundamentals does not yield as sharp a sensitivity measure as do the partial variances since the integrand of the average $\langle \partial f/\partial u_\ell \rangle$ is not necessarily a positive function and consequently could erroneously indicate a small sensitivity by fortuitous cancellation in different regions of parameter space. The partial variances are not subject to this difficulty; if S_{ω_ℓ} is zero or smaller it is definitely due to lack of sensitivity of the output to the ℓ'th parameter.

I. Relation to Linear Sensitivity Analysis

We discuss here the relationship of our nonlinear method of sensitivity analysis to the more usual methods of linear sensitivity analysis. In the linear methods one computes, one way or another, the derivatives $dc/du_{\ell}|_{\underline{u}=0}$ for $\ell=1,2,\ldots,n$. This validity of this procedure must certainly be suspect for output functions which deviate significantly from linearity in the uncertainties in one or more of the parameters. It is thus clearly of interest to investigate the conditions under which our Fourier amplitude analysis reduces to the linear analysis.

To demonstrate this relationship, we express the average

$$\langle f(\underline{x})\rangle \equiv \int \cdots \int d\underline{x}\; p(\underline{x}) f(\underline{x}) \tag{2.32}$$

of a function $f(\underline{x})$ in terms of the Taylor series expansion of $f(\underline{x})$. The multivariate probability distribution function $p(\underline{x})$ can be written formally as

$$p(\underline{x}) = \sum_{\{\mu\}} m_{\{\mu\}} \prod_{i=1}^{n} \frac{(-1)^{\mu_i}}{\mu_i!}\, \delta^{(\mu_i)}(x_i) \tag{2.33}$$

where $\delta^{(\mu_i)}(x_i)$ is the μ_i'th derivative of the Dirac delta function with respect to its argument,

$$\sum_{\{\mu\}} \equiv \sum_{\mu_1=0}^{\infty} \sum_{\mu_2=0}^{\infty} \cdots \sum_{\mu_n=0}^{\infty}$$

and where

$$m_{\{\mu\}} = \left\langle \prod_{j=1}^{n} x_j^{\mu_j} \right\rangle \tag{2.34}$$

are the multivariate moments of $p(\underline{x})$. Using this expression for $p(\underline{x})$ in

Eq. (2.32) yields

$$\langle f(\underline{x}) \rangle = \sum_{\{\mu\}} m_{\{\mu\}} \left[\left(\prod_{i=1}^{n} \frac{1}{\mu_i!} \frac{\partial^{\mu_i}}{\partial x_i^{\mu_i}} \right) f(\underline{x}) \right]_{\underline{x}=0} \tag{2.35}$$

This is the desired relationship between the average of a function of a set of variables and the coefficients of the Taylor series expansion of the function.

This analysis is readily applicable to the probability distributions and output functions discussed in the previous sections. Let us choose, for instance, the probability density

$$P(\underline{u}) = \prod_{j=1}^{n} a_j / \cosh (a_j u_j)$$

of eq. (2.31) with moments

$$m_{\{2\mu+1\}} = 0$$

$$m_{\{2\mu\}} = \sum_{i=1}^{n} \left(\frac{\pi}{2a_j} \right)^{2\mu_i} |E_{2\mu_i}| \tag{2.36}$$

where E_K is the Euler number of index K. The output function in $\underline{u}$-space which we will consider is

$$f(\underline{u}) = \frac{2}{a_\ell} \frac{\partial f(\underline{u})}{\partial u_\ell} \tag{2.37}$$

since, by Eq. (2.30), the average of this function with the probability density $P(\underline{u})$ of Eq. (2.31) yields the Fourier coefficient B_{ω_ℓ}, i.e.

$$\frac{2}{a_\ell}\left\langle\frac{\partial f(\underline{u})}{\partial u_\ell}\right\rangle = B_{\omega_\ell} = \sum_{\{\underline{\mu}\}}\left[\left(\prod_{i=1}^{n}\Gamma_{2\mu_i}\frac{\partial^{2\mu_i}}{\partial u_i^{2\mu_i}}\right)\frac{2}{a_\ell}\frac{\partial f(\underline{u})}{\partial u_\ell}\right]_{\underline{u}=0} \tag{2.38}$$

with

$$\Gamma_{2\mu_i} = \frac{|E_{2\mu i}|}{(2\mu_i)!}\left(\frac{\pi}{2a_i}\right)^{2\mu_i} \propto \left(\frac{1}{a_i}\right)^{2\mu_i} \tag{2.39}$$

Substitution of Eq. (2.39) into (2.38) then leads to the desired result

$$B_{\omega_\ell} = \frac{2}{a_\ell}\left.\frac{\partial f(\underline{u})}{\partial u_\ell}\right|_{\underline{\omega}=0} + \sum_{\{\underline{\mu}\}}{}' \left[\left(\prod_{i=1}^{n}\left(\frac{1}{a_i}\right)^{2\mu_i}\frac{\partial^{2\mu_i}}{\partial u_i^{2\mu_i}}\right)\frac{2}{a_\ell}\frac{\partial f(\underline{u})}{\partial u_\ell}\right]_{\underline{u}=0} \tag{2.40}$$

where the prime on the μ sum excludes the $\mu_1 = \mu_2 = \ldots = \mu_n = 0$ term.

In order for linear sensitivity analysis to be valid, the higher order terms of Eq. (2.40) must be small compared to the first, i.e. the linear, term. These higher order terms will be small only if the output function is essentially linear in the uncertainties of all the parameters. The validity of a linear sensitivity analysis can therefore not be established until some evaluation or estimation of these higher order terms has been carried out. Our Fourier amplitudes, as shown in Eq. (2.40), do include the effects of the higher order terms and therefore represent nonlinear sensitivity measures.

The results of this section can easily be transcribed to show that the partial variances, S_{ω_ℓ}, as defined in Eqs. (2.25) and (2.26), are also <u>non-linear</u> sensitivity measures which include the effects of the higher terms of the expansion (2.40). This is readily evident from the definition of the variances σ^2 and σ_ℓ^2 in terms of the Fourier amplitudes, Eqs. (2.23) and (A4.2).

III. Implementation

The sensitivity coefficients are given by sums of the solutions of the equation set at selected points in the uncertainty space. From the point of view of computation, all that is required is the solutions of the equation set for different combinations of the parameters $(k_1, k_2, \ldots k_n)$. The analysis of section II shows which combinations of solutions to sum and interprets the sum as a sensitivity coefficient.

The parameters are varied simultaneously by relating them to a search variable s and a frequency set $\underline{\omega} = (\omega_1, \omega_2 \ldots \omega_n)$ as given in Eqs. (2.2) and (2.5), i.e.

$$k_\ell = g_\ell[G_\ell(\sin\omega_\ell s)] \qquad (\ell=1,2,\ldots n). \tag{3.1}$$

The frequency ω_ℓ and transformation functions G_ℓ are chosen such that the path in $\underline{k}$-space induced by varying s traverses $\underline{k}$ space in accordance with the probability density $P_\ell(u_\ell)$ representing the uncertainty in each parameter k_ℓ. As long as $\underline{k}$ and s space averages are properly connected, sensitivity coefficients can be calculated as s-space, i.e. one dimensional, quadratures.

The appropriate s-space averages to calculate are the s-space Fourier coefficients defined in Eq. (2.8). The analysis of section II demonstrates that the combination of Fourier coefficients which we call the partial variances

$$S^{(i)}_{\omega_\ell} = \frac{\sum_p (|A^{(i)}_{p\omega_\ell}|^2 + |B^{(i)}_{p\omega_\ell}|^2)}{\sum_j (|A^{(i)}_j|^2 + |B^{(i)}_j|^2)} \tag{3.2}$$

measure the sensitivity of the ith variable to the uncertainty in the ℓ'th parameter. The sensitivity coefficient $S^{(i)}_{\omega_\ell}$ is that part of the variance

of the ith output which arises from the uncertainty in the ℓ'th parameter when the output is averaged over the uncertainties in all other parameters (cf. section IIG).

The Fourier coefficients can be calculated if solutions of the equation set eq. (2.1) are known for values of $\underline{k}$ prescribed by the transformation functions G_ℓ and frequencies $\underline{\omega}$. Since we assume that the reader has available a method of solution of the equation set, all that need be done to obtain the sensitivity coefficient is to "add" the solutions according to Eq. (3.2).

Implementation of the above scheme on a computer requires certain compromises which lead to approximations to the sensitivity coefficients. We have shown in section II that these approximations are controllable; here we investigate their impact on the numerical calculation of the sensitivity coefficients.

In brief, we are replacing a multidimensional integral over the uncertainty space (the $\underline{k}$ space) by a quadrature formula which is a sum over N points in $\underline{k}$ space. The quadrature requirements fall loosely into three areas: 1) use of integer frequencies $\underline{\omega}$; 2) use of a finite number of points N; 3) the choice of frequencies ω. We now discuss these issues in turn.

1. Integer Frequencies

If the search curve is to come arbitrarily close to every point in $\underline{k}$ space, the frequencies Ω_i that define this curve must be incommensurate:

$$\sum_{i=1}^{n} r_i \Omega_i \neq 0 \qquad (r_i\text{'s integer}) \tag{3.3}$$

A consequence of this condition is that at most one of the frequencies can be rational, with all others being irrational. But a computer can only represent an irrational number approximately. Of course, the difference between the irrational and its rational approximation can be made smaller

and smaller by resorting to representations of successively higher precision. But eventually, one will run out of computer memory, so that there is a real limit to the accuracy of the representation.

Once we accept the limitations of rational approximation of irrational numbers, we realize that the frequency set as represented on the computer cannot be truly irrational. It therefore becomes necessary to define a sequence of approximations to incommensurability. This was done in the previous papers[1,2,3] as follows:

A set of rational numbers Ω_i $(i = 1,2,\ldots n)$ is <u>approximately incommensurate to order M</u> if

$$\sum_{i=1}^{n} r_i \Omega_i \neq 0$$

for (3.4)

$$\sum_{i=1}^{n} |r_i| \leq M + 1$$

with M an integer at our disposal. It should be clear from this definition that incommensurability corresponds to $M \to \infty$.

Henceforth we assume that the frequencies are approximately incommensurate to order M.

If we are now dealing with rational numbers we may as well take them to be integers. The correspondence between the rationals Ω_ℓ and integers ω_ℓ is simple to establish with the introduction of ω_L, the least common integer multiple: ω_L is defined as the smallest integer such that

$$\omega_\ell = \omega_L \Omega_\ell \qquad (\ell = 1,2,\ldots n) \tag{3.5}$$

are integers for all ℓ.

The search curve with $\underline{\omega}$ integer, Eq. (3.1), is a <u>closed</u> curve in <u>k</u>

space since for s outside the range $(-\pi,\pi)$, u_ℓ must repeat a value from the range $(-\pi,\pi)$.

The total arc length of the closed search curve defined above will increase with increasing M, the order of incommensurability. Thus, eq. (3.4) serves to define a sequence of approximate search curves which successively become more nearly space filling as $M \to \infty$.

We must balance the increased accuracy which one obtains by using a longer search curve against the increasing computation time required to evaluate the output functions for more of the $\underline{k}$ space.

2. Discrete Sampling

The search curve given in eq. (3.1) does not yet completely fix a sample of parameter space which can be utilized in real problems because the number of points on the search curve is uncountably infinite. We must select a finite subset of these points in constructing an actual sample. Such a selection might be made in many possible ways. The simplest choice, and the only one we have investigated to date, is to take a set of points uniformly spaced along the closed search curve. We require that one of these points lies at s = 0, since s = 0 is that point for which all parameters k_ℓ take on their nominal values $k_\ell^{(o)}$.

The minimum number of points we must take in our sample can be related to the maximum frequency ω_{max} of the frequency set. This relation can be derived by appeal to Nyquist's criterion for the evaluation of Fourier coefficients[15]. We want to evaluate all complex Fourier coefficients C_j for the frequency range

$$0 \leq |j| \leq 2\omega_{max} \quad . \tag{3.6}$$

There are a total of $4\omega_{max} + 1$ such coefficients. By Nyquist's criterion, at least $4\omega_{max} + 1$ points must be taken on the search curve in order to be able to evaluate this number of coefficients.

It also is convenient to let the number of points be even. We therefore let $N = 2r\ (\geq 4\omega_{max} + 2)$ be the number of uniformly spaced sample points along the search curve, and define

$$s_j = \frac{\pi(j-r)}{r} \qquad (j = 1,2,\ldots 2r) \quad . \tag{3.7}$$

Furthermore, if we choose the frequencies ω_i to be <u>odd</u> integers it is easy to show (Appendix 5) that the output function, as a function of s, exhibits the symmetries

$$\begin{aligned} f(\pi/2 + s) &= f(\pi/2 - s) \\ f(-\pi/2 - s) &= f(-\pi/2 + s) \end{aligned} \tag{3.8}$$

so that the search variable's range may be restricted to $-\pi/2 \leq s \leq \pi/2$. Thus, it is sufficient to evaluate $f(s_j)$ only for those s_j which satisfy

$$-\pi/2 \leq s_j \leq \pi/2. \tag{3.9}$$

The number of points which satisfy this criterion is r instead of 2r.* If we choose 2r to be of the form 4q + 2 with q integer, i.e. divisible by two but not by 4, then eq. (3.7) can be modified to

$$s_j = \frac{\pi(j-r)}{r} \quad ; \; j = \frac{r+1}{2}, \frac{r+3}{2}, \ldots, \frac{3r-3}{2}, \frac{3r-1}{2}, \tag{3.10}$$

or, more conveniently,

$$s_\ell = \frac{\pi}{r}\left(\frac{2\ell-r-1}{2}\right) \; ; \quad \ell = 1, 2, \ldots, r \quad . \tag{3.11}$$

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* In references (1), (2), and (3), this symmetry was not invoked, so that the number of sample points listed in these papers are all too large by a factor of two.

Aside from a lower limiting value* $r \geq 2\omega_{max} + 1$, fixed by the Nyquist criterion, r can be assigned any value. However, large values of r are numerically desirable for reasons of accuracy, although smaller values are desirable for reasons of computing economy. To date, in practical applications we have tended to allow considerations of economy to prevail, and we usually have chosen $r = 2\omega_{max} + 1$.

It is important to realize that a more accurate evaluation of the Fourier coefficients, made possible by choosing r to be large, may not result in improved accuracy for the sensitivity coefficients. For, if the search curve does not do an adequate job of covering the parameter space, then increasing the accuracy of the s-space integration will not improve the coverage of the parameter space. Thus, in addition to insuring that r is sufficiently large to obtain an accurate s-space quadrature, we must also investigate how to obtain an s-space curve which does a good job of covering the entire parameter space.

3. Selection of Frequency Set

An adequate coverage of the parameter space is ensured by an appropriate choice of the integer frequencies ω_i and the number of points 2r. Criteria for such a choice were discussed in references (1) and (2) and sets of $\underline{\omega}$,N (N=2r) generated according to these criteria are presented there. Note that once a set has been constructed for n parameters, this same set can be used in all n parameter problems; i.e., frequency sets can be tabulated once and for all.

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* In reference (1), it is indicated that by appropriately choosing the frequency set ω_ℓ it is possible to use a slightly smaller lower limit value for r, $r=2\omega_{max} - 7$. The practical difference between these two limits is small, and we prefer to use the larger value for purposes of discussion. In actual calculations, we have used both values.

For a given choice of frequency set $\underline{\omega}$ and number of points 2r we obtain an approximate sensitivity coefficient which we designate by an asterisk. Thus, we can write

$$A_\ell^* = A_\ell + \varepsilon_\ell(\underline{\omega}, 2r) \tag{3.12}$$

where A_ℓ is the true Fourier coefficient, A_ℓ^* the calculated Fourier coefficient and ε is the error, which depends on $\underline{\omega}$, 2r and the index ℓ of the coefficient to be calculated.

The analysis of reference (3) and parts of section 2 of this paper address the difficult problem of how to determine what the error is under given circumstances and how to minimize this error by properly choosing 2r and $\underline{\omega}$. For the purpose of presentation of this implementation, we assume that the error has been made sufficiently small to carry out a meaningful sensitivity analysis.

4. Working Equations

The symmetries exhibited in eq. (3.8) simplify the computation of the numerical Fourier coefficients. If we recall that the total number of points 2r is chosen as 4q+2 with q an integer, the use of these symmetries leads to (see Appendix VI)

$$A_\ell^* = 0 \qquad (\ell \text{ odd}) \tag{3.13a}$$

$$B_\ell^* = 0 \qquad (\ell \text{ even}) \tag{3.13b}$$

$$A_\ell^* = (2q+1)^{-1}\left\{f_0 + \sum_{j=1}^{q} (f_j + f_{-j}) \cos\frac{\pi \ell j}{2q+1}\right\} \qquad (\ell \text{ even}) \tag{3.13c}$$

$$B_\ell^* = (2q+1)^{-1}\left\{\sum_{j=1}^{q} (f_j - f_{-j}) \sin\frac{\pi \ell j}{2q+1}\right\} \qquad (\ell \text{ odd}) \tag{3.13d}$$

where we have set $f(s_j) = f_j$. These formulae generate q+1 unique cosine coefficients and q unique sine coefficients. They form the working formulae of our method, whereby we use the sample values f_j for $-q \leq j \leq q$ to generate the Fourier coefficients.

We might particularly note that Eq. (3.13c) gives, for $\ell = 0$

$$A_0^* = (2q+1)^{-1} \sum_{j=-q}^{q} f_j \tag{3.14}$$

identifying A_0^* as the mean value of f(s). The variance of f is generated by the formula

$$\sigma_f^2 = (2q+1)^{-1} \sum_{j=-q}^{q} (f_j - A_0^*)^2 \tag{3.15}$$

It is worth pointing out that in any practical calculations, the amount of computing needed for evaluating Fourier coefficients is a very small part of the total computing. No significant benefit is thus gained by attempting to introduce methods such as Fast Fourier Transforms (FFT) into the analysis. There would in fact appear to be disadvantages in using FFT in this application, since FFT works best when the numbers of sample points is highly composite, e.g., a number of the form of 2^n, whose n is some integer, whereas our analysis gains in simplicity when the number of points is not highly composite.

5. A Useful Modification

Under certain circumstances, partial information may be available concerning the dependence of an output function upon one or more of the parameters. It may be possible to use this information to improve the numerical accuracy of the computation of the partial variances. By way of example, suppose we knew that a particular output function f was an <u>even</u> function of a particular parameter, say k_1, i.e., $f(-k_1) = f(k_1)$. In such a case it is easy to establish that the Fourier fundamental of frequency ω_1, and all odd harmonics, vanish identically. However, even harmonics would not in general vanish. If we were to compute on the basis discussed previously, half of the terms contributing to the partial sensitivity would vanish, including the fundamental -- for which we might otherwise expect higher numerical accuracy than for the even harmonics.

To circumvent this loss of accuracy, we can utilize the following trick. We define a new parameter k_1' by

$$k_1' = k_1^2 \tag{3.16}$$

with a distribution function $P_1'(k_1')$ related to $P_1(k_1)$ by

$$P_1'(k_1') = P_1(k_1) \frac{dk_1}{dk_1'} = \frac{P_1(\sqrt{k_1'})}{2\sqrt{k_1'}} \quad . \tag{3.17}$$

We then utilize k_1' and $P_1'(k_1')$, instead of k_1 and $P_1(k_1)$, to determine G_1 by Eq. (2.6). Finally, k_1' instead of k_1 is related to s <u>via</u> Eq. (3.1).

With this modification, the fundamental Fourier coefficient B_{ω_1}, and in general all of the harmonic coefficients do not vanish, and we can expect a more accurate evaluation of the partial variance.

In a more general vein, suppose we have a priori knowledge, or suppose we have qualitative reason to believe, that the output function f depends upon k_1 via an explicit function of k_1. This is to say, suppose $f(k_1)$ is actually of the form $F(h(k_1))$, with $h(k_1)$ explicit. Then it is best to proceed by defining

$$k_1' = h(k_1)$$

$$P_1'(k_1') = P_1(k_1)\frac{dk_1}{dk_1'} = \frac{P_1(k_1)}{h'(k_1)} = \frac{P_1\left[h^{-1}(k_1)\right]}{h'\left[h^{-1}(k_1')\right]} \quad . \tag{3.18}$$

Next utilize $P_1'(k_1')$ to determine G_1 by Eq. (2.6), and relate k_1' to s by Eq. (3.1). After this, proceed along the lines previously discussed. The use of these modifications can be expected to improve the numerical accuracy of the sensitivity analysis.

IV. Applications

To illustrate the application of our sensitivity analysis method, we present in this section four different examples. The first three of these examples have not been published previously, although two of them are available through government document sources.

The applications to be discussed are the following:

1. An Economic Model
2. A Chemical Laser Model
3. A Socioeconomic Model (World II)
4. A Chemical Reaction Model

In the first of these applications we are dealing with a model which uses linear programming equations. The second and fourth examples deal with models described by ordinary differential equations. The third application involves a set of differential difference equations. Our ability to achieve a successful sensitivity analysis for such different types of model equations demonstrates the wide applicability of our technique of sensitivity analysis.

One important feature should be noted which pervades the analysis of all these examples. A study of the sensitivity coefficients reveals unexpected but significant relations between parameters and output functions which could not have been predicted from a more conventional analysis or a purely intuitive approach. Sensitivity analysis thus provides information which can lead to important insights into the structure of the models used to represent complex systems.

1. AN ECONOMIC MODEL[6]

Frequent use is made of linear programming (LP) and related methodologies in modeling the operation of complex, interacting systems. Generally speaking, the form in which such problems are posed is one of seeking a

constrained optimum to some objective function. Often the objective function is the profit to be derived from a business, and the constraints relate to limitations on available resources, manpower, capital, equipment, and/or demand. There is an enormous literature covering this subject, of which we only cite a few examples.[7] An interesting particular example of application to a model of operation of a petroleum refinery is described in a text by Wilde and Beightler.[8] The structure of this model is such that it can be extended to characterize an aggregated representation of the entire domestic petroleum industry. In this model, a number of crude petroleum producers supply crude oils, each of its own characteristic chemical composition, to a number of refineries, each of specific design. The different crudes each have a range of possible products into which they may be converted, and each refinery has a range of operability with respect to these crudes. For each crude, the supply is limited in an absolute sense by the pumping capacity of the supplier. For each refinery, the process capacity is limited by existing equipment limitations. In addition to these physical constraints, there are economic constraints. The crude suppliers may limit production to below their physical capacity in order to obtain political or economic advantages. The processors may limit production for similar reasons. Furthermore, there may be production limits due to consumers, who at any given time have limitations upon their desire to use or capacity to store products.

All of these factors and others serve to determine the rates of consumption of various crude petroleums, the rates of production of various products, and the rates of consumption of these products. The money flow from consumer to producer to supplier is likewise determined by these factors, as are the profits of the producers and suppliers. Associated with many of these factors are numerical values of parameters, almost all of which are imprecisely known. Furthermore, these parameters are not static but tend to fluctuate in time, both in response to factors internal to the petroleum industry, and to socioeconomic, political, and technical factors external to the petroleum industry. These fluctuations make profit optimization difficult, and make performance prediction for the industry equally difficult.

The objectives of our study[6] were to develop a simple aggregated model of industry economics, apply sensitivity analysis to the model, and to see whether the resulting methodology might be useful as a means of determining which parameters most influence costs, profits, and the development of shortages.

The mathematical structure of the model is as follows: The symbol x_{ik} denotes the daily national utilization of crude petroleum available from source i and which is converted to products by process k. The physical constraints of supply can be written as

$$\sum_k x_{ik} \leq b_i \quad (i = 1, 2, \ldots, N) \tag{4.1}$$

where b_i is the availability of type i crude. The constraints of consumer demand are of the type*

$$\sum_{i=1}^{N} \sum_k a_{jik}\, x_{ik} \leq b_{N+j} \quad (j = 1, 2, \ldots, M) \tag{4.2}$$

*The meaning of this relation is that production will not exceed demand. Clearly this relation is not instantaneously true, but rather represents a time average. That is, at any given instant, production may well exceed demand, but over the long term, either demand will increase (perhaps due to price adjustments) or production will be reduced so as to restore a condition in which the inequality (4.2) is satisfied.

where a_{jik} is the amount of product j produced from crude i by process k, and b_{N+j} is the consumer demand for product j.

The production industry tries to operate so as to optimize the daily* profit P, which is given by

$$P = \sum_{j=1}^{M} y_j s_j - \sum_{i=1}^{N} x_i p_i \,, \tag{4.3}$$

where

$$x_i = \sum_k x_{ik} \,, \tag{4.4}$$

and where s_j is the selling price of product j, y_j is the daily production of product j, x_i is the daily production of crude i, and p_i is the cost of crude i. The latter cost includes the cost of transportation to the refinery, and an allocated cost of shipping to the consumer for each product manufactured from crude i at the refinery. Production and utilization are related by

$$y_j = \sum_{i=k}^{N} \sum_k a_{jik}\, x_{ik} \,, \tag{4.5}$$

so that by substitution

$$P = \sum_i \sum_k \left[-p_i + \sum_j s_j\, a_{jik} \right] x_{ik} \tag{4.6}$$

*We use in general one day as the unit of time, one barrel as the unit of production, both of crudes and of products, and one dollar as the unit of profit or loss.

For a given set of prices s_i consumer demand will vary. Although the finer details of this variation may be obscure, it is plausible to model this variation by the relations

$$b_{N+j} = g_j \left[1 - \left(\frac{s_j}{s_{ju}}\right)^{q_j}\right] \tag{4.7}$$

where g_j is the limiting consumer demand as the price falls to zero, and s_{ju} is the limiting upper price at which demand falls to zero.* The exponent q_j fixes the marginal demand, i.e., the rate of change of demand with respect to price. Small values of q_j are referred to as indicating large elasticity of demand, and large values of q_j are referred to as indicating small elasticity of demand. For essential goods, such as many petroleum products, q_j tends to be large (i.e., $>> 1$). The specific values of g_j, s_{ju} and q_j for a given product must be regarded as experimental parameters which can only be determined by observations of the response of the market place to price changes. In addition, they are not truly constants for any product, but display variations in time due to changes in technology, social structure, political institutions, public policies and other factors.

If we substitute Eq. (4.7) into Eq. (4.2), we are then confronted with the problem of maximizing P as a function of the prices s_j and the production levels x_{ik}, subject to the

*Equation (4.7) is an approximate form which should not be interpreted as literally valid over too broad a range of s_i. If product i is an essential material, nations will go to war at prices well below $s_i = s_{iu}$, if war promises to induce a cheaper supply. Also, even if s_i were to approach zero, demand does not become infinite because of limits in consumer's storage capacity.

nonlinear constraints, Eq. (4.2), and the linear constraints Eq. (4.1).* This problem is nonlinear and can be solved. However, we choose instead to introduce a simplification which reduces the problem to a linear one. To do this, we require that all products be profitable, a condition we assure by requiring all product prices to equal or exceed the price of the most expensive crude, with a markup to account for processing losses. To state this mathematically, we define

$$\hat{a}_{ik} = 1 - \sum_{j} a_{jik} , \qquad (4.8)$$

that is, $\hat{a}_{ik}$ is the fraction of each barrel of crude i lost during production by process k. Then define a lower price level s_ℓ by

$$s_\ell = \max_{i,k} \frac{p_i}{(1-\hat{a}_{ik})} \quad (j = 1, 2, \ldots, N) \qquad (4.9)$$

Sale of any product at a price (per barrel) in excess of s_ℓ will be profitable.

Define then a parameter λ_i for each product such that its price is given by

$$s_i = s_\ell + \lambda_i (s_{iu} - s_\ell). \quad (i = 1, 2, \ldots, M) \qquad (4.10)$$

Then if $\lambda_i = 0$, we have $s_i = s_\ell$; but if $\lambda_i = 1$, we have $s_i = s_{iu}$, the limiting upper price at which sales of product i would fall to zero.

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*This statement views the problem from the point of view of the refiners. In reality, the problem is more complex, because the producers interest is in maximizing his profit (which is not expressed by Eq. (4.6)) subject to the constraints. The producer's tool for attempting this is by variation of the crude prices p_j, analysis of which presents a more complex problem than that we will consider here.

Clearly then each λ_i must fall into the range* $0 \leq \lambda_i \leq 1$. We can refer to the λ_i's as the "markup parameters" for the products, and utilize the λ_i's as equivalent to a representation of the prices s_i.

We can develop an analysis in which the λ_i's are varied independently of the crude prices p_j. If we then consider a fixed set of λ_i's, the prices and hence the consumer demand constraints, Eq. (4.2), will be determined via Eqs. (4.7) - (4.10). Then for a fixed set of supply constraints, Eq. (4.1), the profit optimization problem reduces to a linear programming problem, namely that of maximizing P subject to the linear constraints of Eqs. (4.1) and (4.2). The form of this problem is essentially the same as that discussed by Wilde and Beightler.[8]

We now have defined a linear programming problem in which producer's seek to maximize the total profit P, Eq. (4.6) for given values of crude prices p_j, crude availabilities b_j, product saturation demands q_i, product cutoff prices s_{iu}, product markup rates λ_i and demand exponents q_i. None of these parameters are constants, but rather they all vary from time to time in response to social, economic and psychological forces. It is important to try to understand how the variability of supply and price will influence costs, consumptions,

*It is implicit that $s_\ell \leq \min_i s_{iu}$, which effectively states that we consider only the economic circumstances in which producer prices are not set so high as to prevent sales of any product because of the impact of Eq. (4.7).

and shortages of refined products. Markup rates are subject to fluctuation. Saturation demands, cutoff prices, and demand exponents are only measurable approximately, and furthermore fluctuate in time. Thus we have an LP problem with a large number of parameters of uncertain value. The problem solution depends upon these parameter values. What we have done is to treat these parameter uncertainties statistically, thereby generating a set of linear programming problems. We have performed a sensitivity analysis and determined which parameter uncertainties are most influential in causing variability in the following dependent variables: product consumptions, crude consumptions, expenditures for crudes, expenditures for products, profits and unfilled demands, i.e., shortages.

In the study that was performed, only a subset of the parameters was taken to be uncertain: crude prices, product markup rates and the demand exponent. It was furthermore assumed that the demand exponent was the same for all products, i.e.,

$$q_i = q \quad (i = 1, \ldots, M) \tag{4.11}$$

Other parameters were given constant values (i.e., no uncertainty was assumed) based upon a brief analysis of data on petroleum economics. The range of prices was such that price and not physical supply constrained production.

To illustrate application of the methodology, an aggregated model was chosen in which there are four types of

crudes available. Of these, three could be processed only in one way, and the fourth had two alternative processes applicable to it. The crude production variables then are labeled x_{11}, x_{21}, x_{31}, x_{41}, and x_{42}. Products were put into four classifications, termed "gasoline" (subscript = 1), heating oil (subscript = 2), lubricating oil (subscript = 3), and aviation fuel (subscript = 4). Available crude supplies, product saturation demands and product cutoff prices are given in Table 4.1. The coefficient matrix a_{jik} is given in Table 4.2.

The ranges of the parameter values are shown in Table 4.3. Because we did not have statistical data on the probability distribution of these parameters, we in all cases assumed a uniform distribution between the indicated lower and upper limits. All of the parameter ranges were based upon rough estimates derived from real data. The crude prices quoted in Table 4.3 includes costs of transportation to the refinery, costs of product transportation to the retail market, and costs of processing. The sum of these costs is about $5.00/barrel, so that the range of wellhead prices which corresponds to Table 4.3 is about $7.00 to $11.00/barrel ($5.00 to $10.00/barrel for Type 3 crude).

With nine uncertain parameters, it is necessary to solve 323* linear program problems, using 323 parameter sets, as

*According to reference 2, 630 problems must be solved, but the two-fold symmetry discussed in Section III reduces this to 315 problems. The slightly higher value 323 is obtained from the relation $N = 2N_{max}+1 = 2(161) + 1 = 323$.

TABLE 4.1

CONSTRAINTS AND PARAMETERS OF A TEST PROBLEM IN PETROLEUM ECONOMICS

Available Crude Supplies

$b_1 = 7.0 \times 10^6$ barrel/day

$b_2 = 7.0 \times 10^6$ barrel/day

$b_3 = 7.0 \times 10^6$ barrel/day

$b_4 = 4.2 \times 10^6$ barrel/day

Product Saturation Demands

$g_1 = 9.8 \times 10^6$ barrel/day

$g_2 = 4.9 \times 10^6$ barrel/day

$g_3 = 6.0 \times 10^5$ barrel/day

$g_4 = 2.1 \times 10^6$ barrel/day

$s_{1u} = \$42.00$/barrel

$s_{2u} = \$46.00$/barrel

$s_{3u} = \$180.00$/barrel

$s_{4u} = \$60.00$/barrel

TABLE 4.2

MATRIX OF REFINERY CAPACITY COEFFICIENTS a_{jik}

j \ ik	11	21	31	41	42
1	0.6	0.5	0.4	0.6	0.5
2	0.2	0.3	0.4	0.3	0.1
3	0.0	0.0	0.0	0.0	0.2
4	0.1	0.1	0.1	0.0	0.1

TABLE 4.3

RANGE OF VALUES OF UNCERTAIN PARAMETERS

Crude Prices

p_1	\$12.00/barrel to \$17.00/barrel
p_2	\$12.00/barrel to \$17.00/barrel
p_3	\$10.00/barrel to \$15.00/barrel
p_4	\$12.00/barrel to \$17.00/barrel

Product Markup Parameters

λ_1	0.03 to 0.07
λ_2	0.03 to 0.07
λ_3	0.03 to 0.07
λ_4	0.02 to 0.04

Product Markup Exponent

q	5.9 to 6.1

defined by Eq. (3.1). The nine frequencies ω_i are given in Table I of reference (2). A computer program was written which selects parameter sets and which then calls on a standard linear programming subroutine to solve a problem. The results are then collected and transformed by the main program so as to provide mean values, $\langle f \rangle$, variances σ_f^2 and partial variances $S^*_{\omega_\ell}$ (c.f.) Eqs. (3.2) and (3.15). The output functions studied were the consumption rates for the individual crude petroleums, the daily expenditures for all crudes, and for all products, the daily profits of the refineries, the daily deliveries of the products and the unfilled demands. Tables 4.4, 4.5, and 4.6 summarize the results.

In Table 4.4 we consider the variables x_i (c.f., Eq. (4.4)), the consumptions of the four crude petroleums. For each crude, the table lists the available supply. Also listed are the minimum and maximum consumption as obtained from the sample of 323 calculations. In all cases these vary from the maximum available down to zero. The nominal consumptions correspond to the single choice $s = 0$ for the search variable. For a uniform probability distribution this means that all variables have been taken as the average value in their ranges of uncertainty (c.f., Table 4.3). The coefficient of variation v_f provides an alternative representation of the variance. By definition the coefficient of variation, v_f, of a random variable f is given by

$$v_f = \sigma_f / \langle f \rangle \tag{4.12}$$

TABLE 4.4

SENSITIVITY ANALYSIS OF CONSUMPTIONS OF CRUDE OILS, DAILY EXPENDITURES, AND PROFIT RATES

	Crude Consumptions (bbl/day)			
	Crude Type 1	Crude Type 2	Crude Type 3	Crude Type 4
Available Supply	7.0×10^6	7.0×10^6	7.0×10^6	4.2×10^6
Minimum Daily Consumption	0	0	0	0
Nominal Daily Consumption	7.0×10^6	1.3×10^6	7.0×10^6	3.0×10^6
Average Daily Consumption	4.7×10^6	3.3×10^6	6.1×10^6	3.6×10^6
Maximum Daily Consumption	7.0×10^6	7.0×10^6	7.0×10^6	4.2×10^6
Coefficient of Variation v_f	0.686	0.921	0.249	0.202
Partial Variances $S^*_{\omega_\ell}$				
Price of Crude No. 1 (p_1)	0.422	0.124	0.025	0.012
Price of Crude No. 2 (p_2)	0.197	0.567	0.275	0.247
Price of Crude No. 3 (p_3)	0.022	0.039	0.252	0.001
Price of Crude No. 4 (p_4)	0.004	0.011	0.001	0.398
Markup of Product 1 (λ_1)	0.004	0.000	0.003	0.006
Markup of Product 2 (λ_2)	0.001	0.000	0.000	0.001
Markup of Product 3 (λ_3)	0.004	0.001	0.000	0.002
Markup of Product 4 (λ_4)	0.004	0.001	0.001	0.002
Product Markup Exponent (q)	0.003	0.001	0.006	0.003

The data in Table 4.4 indicates considerable variability in consumption of the individual crudes as a consequence of changes in the parameters. The partial variances indicate the differing degree to which parameter uncertainties contribute to consumption variability. We briefly summarize the much longer discussion of results contained in the report by Levine.[6] First, it is not surprising that consumption of Crude Type 1 is more sensitive to variation in the price of Crude Type 1 than it is in any other variable. The only other variable of importance in this regard is the price of Crude Type 2. Similarly, consumption of Crude Type 2 is most sensitive to the cost of Crude Type 2. However, when we come to Types 3 and 4 Crude the situation is different. Consumption of Type 3 is more dependent upon price of Type 2 than on its own price, and consumption of Type 4 is nearly as sensitive to the price of Type 2 as it is to its own price. These latter relations suggest a tendency for Type 2 to serve as a substitute for Types 3 and 4 under certain conditions of relative price.

In Table 4.5 we consider costs of crudes and of products, and refinery profits. The table clearly indicates that the net expenditures for all crude petroleum is more sensitive to the price of Type 3 Crude than to any other parameters, somewhat less sensitive to the price of Type 2 Crude, and comparatively insensitive to the other parameters. This conclusion with respect to Type 3 Crude is in accord

TABLE 4.5

SENSITIVITY ANALYSIS OF EXPENDITURE RATES FOR CRUDE PETROLEUMS, EXPENDITURE RATES FOR REFINED PRODUCTS, AND REFINERY PROFITS
(Units: Dollars/Day)

	Expenditures for Crude Petroleum	Expenditures for Refined Products	Profit
Minimum	1.583×10^8/day	2.301×10^8/day	2.864×10^7/day
Nominal	2.511×10^8	2.915×10^8	4.046×10^7
Average	2.358×10^8	3.027×10^8	6.695×10^7
Maximum	2.827×10^8	3.488×10^8	1.119×10^8
Coefficient of Variation v	0.098	0.076	0.243
Partial Variances $S^*_{\omega_\ell}$			
Price of Crude No. 1	0.070	0.043	0.071
Price of Crude No. 2	0.169	0.328	0.112
Price of Crude No. 3	0.375	0.059	0.287
Price of Crude No. 4	0.065	0.133	0.059
Markup of Product 1 (λ_1)	0.006	0.040	0.030
Markup of Product 2 (λ_2)	0.001	0.009	0.010
Markup of Product 3 (λ_3)	0.007	0.012	0.003
Markup of Product 4 (λ_4)	0.002	0.002	0.000
Product Markup Exponent (q)	0.006	0.006	0.001

with the data in Table 4.4, which shows the daily average consumption of Type 3 Crude to be higher than that of any other crude, either on an absolute or a relative basis. Less obvious is the ranking of the price of Type 2 Crude as the second most important parameter, particularly when one notes that its daily average consumption is the least of all of the crudes. We also note from Table 4.4 that the coefficient of variation is higher for the consumption of Type 2 than it is for any other crude, so that its average consumption represents the mean value of a widely dispersed variable.

The observation of the importance of the price of Type 2 Crude as a parameter is a good illustration of the ability of sensitivity analysis, in the form we have developed, to locate obscure but significant relationships. By contrast, if we had only considered nominal parameter values, or small variations about nominal parameter values, we would have found the nominal daily consumption of Type 2 Crude to be the least of all the crudes (see Table 4.4), and we likely would have concluded that its price did not importantly affect net expenditures. Sensitivity analysis thus gives us clues which, if pursued, can lead to deeper insights into the structure of a complex system than we could obtain by more conventional analysis.

In the same vein, Table 4.5 shows the price of Type 2 Crude to be the most important parameter in the determination of expenditures for refinery products, despite the fact that the average daily consumption of this Crude is less than that of the other Crudes.

It is difficult to provide a simple explanation of the high importance of Type 2 Crude, and the explanation must lie in a complex interplay of the relative prices of the crudes, the different product distributions available from refining different crudes, and the differing product demands. Nonetheless, the fact of this high importance emerges directly from the analysis.

It is perhaps worth remarking on the almost complete insensitivity of the dependent variables to the product mark-ups and the markup exponent. This conclusion is in accord with the real world observation that consumption of petroleum products continues unabated even in the face of large price increases; i.e., the price-demand relation is "highly inelastic", in the language of economics. Petroleum products are simply too important to the consumer for their use to be foregone in virtually all circumstances.

Table 4.6 combines our sensitivity analyses for product delivery rates and for shortages. We can do this in one table because shortage is defined as the algebraic difference between demand and delivery.* Because this relation is linear,

*In constructing Table 4.6, we can define "shortage" in two alternate ways: the difference betweel actual demand at the current price level and delivery; or by the difference between saturation demand and delivery. In practical application to products with an inelastic price demand curve, these two definitions are virtually coincident. This is the situation that applies in this study. For the sake of definiteness, we define shortages relative to saturation demand; i.e., we use the second definition.

TABLE 4.6

SENSITIVITY ANALYSIS OF PRODUCT DELIVERY RATES AND UNFILLED DEMAND (SHORTAGES)

	Product Deliveries and Shortages (Barrels)			
	1	2	3	4
	Gasoline	Heating Oil	Lubricating Oil	Aviation Fuel
Product Saturation Demand (Daily)	9.8×10^6	4.9×10^6	6.0×10^5	2.1×10^6
Minimum Daily Delivery	6.3×10^6	4.1×10^6	0	1.4×10^6
Minimum Daily Shortage	2.0×10^4	6.7×10^3	0	1.9×10^5
Nominal Daily Delivery	9.1×10^6	4.9×10^6	6.0×10^5	1.8×10^6
Nominal Daily Shortage	6.6×10^5	1.5×10^4	0	2.7×10^5
Average Daily Delivery	8.7×10^6	4.9×10^6	5.9×10^5	1.7×10^6
Average Daily Shortage	1.1×10^6	4.2×10^4	1.1×10^4	4.0×10^5
Maximum Daily Delivery	9.8×10^6	4.9×10^6	6.0×10^5	1.9×10^6
Maximum Daily Shortage	3.6×10^6	8.4×10^5	6.0×10^5	7.1×10^5
Coefficients of Variation v_+				
Daily Delivery	0.105	0.022	0.103	0.071
Daily Shortage	0.867	2.539	5.301	0.303
Partial Variances $S^*_{\omega_\ell}$				
Price of Crude No. 1	0.399	0.031	0.017	0.373
Price of Crude No. 2	0.076	0.023	0.072	0.002
Price of Crude No. 3	0.098	0.064	0.009	0.048
Price of Crude No. 4	0.000	0.007	0.079	0.128
Markup of Product 1 (λ_1)	0.008	0.001	0.002	0.004
Markup of Product 2 (λ_2)	0.001	0.003	0.001	0.003
Markup of Product 3 (λ_3)	0.007	0.008	0.018	0.009
Markup of Product 4 (λ_4)	0.004	0.002	0.000	0.002
Product Markup Exponent	0.007	0.015	0.007	0.008

the partial variances of the delivery for a particular product will be the same as the partial variances for the shortages of the same product.

With respect to aviation fuel, the results shown in Table 4.6 indicate that the range of daily deliveries is small, the average and nominal daily deliveries are nearly equal, and the coefficient of variation is small. The price of Type 1 Crude is the most important parameter and the price of Type 4 Crude is the next most important parameter. The rationale for the latter observation is difficult to establish: since all of the Crudes can be used to produce aviation fuel in the same relative proportions, we might expect that the parametric importance would be in the same order as the average daily consumption, but comparison of Tables 4.4 and 4.6 shows this not to be the case. Thus we again see an example where the numerical results of a sensitivity analysis do not conform to those derived by simple reasoning.

With respect to gasoline, a more complex situation arises: there is a moderately large spread of delivery rates, and a corresponding spread of shortages which yields at the upper extreme shortages which are a large fraction ($\sim$ 37 percent) of demand. The only parameter of major significance influencing this variability is the price of Type 1 Crude, despite the fact that it ranks second in average daily consumption.

With respect to heating oil, still another situation arises. The range of daily delivery is small (as reflected

in a small coefficient of variation), but the coefficient of variation of the daily shortage is large. The latter fact stems from the evaluation of shortage as the small difference between two large numbers, demand and delivery . On an absolute basis, the maximum shortage is 17 percent of saturation demand, but the average shortage is less than 1 percent of saturation demand. For this case, the sensitivity analysis does not clearly identify a parameter of maximum importance, and the sum of the partial variances in Table 4.6 is only 0.151, much less than the maximum possible value of unity. This means that the higher order partial variances $\sigma^2_{\ell j}$, $\sigma^2_{\ell jk}$, etc. (c.f., Eqs. (2.28b) and (2.28c)) are important in this case. Although we could calculate these higher order partial variances, we have chosen not to do so, since the relatively low level of shortages renders immaterial such a complicated analysis.

The situation for lubricating oil is similar to that for heating oil, except that the range of daily shortages is even broader, being at the one extreme zero and at the other equal to the product saturation demand. The sum of the partial variances in Table 4.6 is 0.205, again well below unity in value. Here, evaluation of higher order partial variances would be useful, so as to help identify those parameter combinations which induce large shortages.*

*This identification can also be made by direct examination of the 323 sample calculations, which would be a tedious process.

2. A CHEMICAL LASER MODEL[9]

The hydrogen fluoride chemical laser is a chemical system consisting initially of a mixture of molecular hydrogen, H_2, molecular fluorine, F_2, and an inert diluent, e.g., argon. At time t = 0 flashlamp irradiation dissociates some of the F_2 into F atoms. Chain reactions then begin which leads to the conversion of the hydrogen and fluorine into hydrogen fluoride, HF. Because of the high chemical energy release the HF molecules produced are in comparatively high vibrational quantum states. If the system is placed between two mirrors, the vibrational decay will lead to lasing action on the infrared vibration-rotation transitions of the HF molecule. Theoretical descriptions of the system have been provided by various authors.[10,11,12] We have performed a sensitivity analysis on the model of Kerber, Emanuel, and Whittier.[10]

The model studied described the chemical evolution of the system in terms of a set of 68 reversible chemical reactions between the following species: H atoms, Ar atoms, F atoms, $H_2(v)$ molecules, F_2 molecules, $HF(v')$, where v and v' indicate the vibrational quantum states of H_2 and HF, respectively. The model considers the ranges of values $0 \leq v \leq 2$ and $0 \leq v' \leq 8$, so that a total of 16 chemical species are considered. The system is assumed to be spatially homogeneous. Over time-scales of interest it operates adiabatically and at constant volume. Because of the chemical

energy release the temperature is not constant. Except for the Ar atoms, whose number is constant in time, the other 15 chemical species have concentrations which vary in time. Including the temperature variation, the system is described by 16 coupled time-dependent equations, the temperature equation being derived from considerations of energy conservation. For the temperature and for the masses (or number of moles) of all species except HF(v′) the time dependent equation is an ordinary differential equation. The equations for the HF(v′) molecules are of one of two alternate forms. If lasing is not taking place on any transition involving the vibrational level v′, then the equation for that level is an ordinary differential equation, namely an equation of chemical evolution. If lasing is occurring which involves the vibrational level v′ and an adjacent level $v' \pm 1$, then an algebraic relation (the so-called "gain equation") replaces one of the chemical differential equations for the populations of state v′ and state $v' \pm 1$. Thus the system is described in terms of a set of equations in which the equations themselves change form in time. It is not known a priori which equations are applicable at a given time, and auxiliary tests are required in order to determine when changes occur in the equation system.

An important parameter of the system is the "threshold gain", whose value depends upon the reflectivity of the laser mirrors and the spacing between these mirrors. The larger

the value of this threshold gain, the less the system is able to lase. For sufficiently high threshold gain, lasing is completely suppressed. In this case, the equations describing the system become completely "chemical" in form, and consist entirely of coupled ordinary differential equations. The boundary condition on these equations are fixed by the initial chemical composition of the system, the initial pressure and temperature, and (importantly) by the number of fluorine atoms produced by the initiating flashlamp discharge.

The case of complete suppression of lasing action, which is usually termed the "zero-power" case, is therefore relatively simple to treat, and it is also of considerable interest. In particular, it is possible to study the timewise variation of the populations of the HF(v') levels. From this information one can calculate the gains between adjacent levels and determine the times at which lasing would have been initiated had the threshold gain been adjusted to some specific value.

The model is characterized by a very large number of parameters, virtually all of which are known with poor precision. The most significant of these are the 68 rate coefficients, one per reaction,* and the initial conditions of the systems. Preliminary study of the system suggests that

*For each reaction there are <u>two</u> rate coefficients, one forward and one reverse. However, appeal to equilibrium considerations shows that only one of the two is independent, and that the uncertainty in one stands in a fixed relation to the uncertainty in the other. Thus, we can speak of there being one (independent) rate coefficient per reaction.

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only 13 of the 68 rate constants need be studied by sensitivity analysis, and that of the initial conditions, only the initial concentrations of F atoms need be studied. We therefore limited the sensitivity analysis to 14 parameters of the system.

The 13 rate constants which we used in our sensitivity analysis are detailed in Table 4.7. The other rate constants were assumed to stand in certain fixed relations to those listed. The basis for this premise has been discussed by Cohen.[13]

The rate coefficients listed in Table 4.7 are temperature dependent. Broadly speaking, the values in Table 4.7 are more reliable near 300°K (where they have been studied experimentally) than at higher temperatures, where numerical evaluation is based upon extrapolation of measurements beyond the range of experimental study. In principle, sensitivity analysis could study the separate influences of uncertainties in the absolute value of the rate coefficients at a fixed temperature within the experimental range (i.e., a pre-exponential or temperature independent factor), and the influence of uncertainties in the temperature dependent part of the rate constant (i.e., the activation energy). Such a separation into temperature independent and temperature dependent uncertainties was not undertaken in the referenced study. Instead, at the suggestion of N. Cohen[14]

TABLE 4.7

SOME RATE COEFFICIENTS OF THE HF CHEMICAL LASER[9],[10]

Index	Reaction	Rate Coefficient*
1	$H + H + M_2 \rightleftarrows H_2(0) + M_2$	$10^{18}\ T^{-1.0}$
2	$F_2 + M_4 \rightleftarrows F + F + M_4$	$5.0 \times 10^{13}\ \exp(-17765/T)$
3	$HF(v) + M_4 \rightleftarrows H + F + M_4$	$1.2 \times 10^{19}\ T^{-1.0}\ \exp(-68334/T)$
7	$F + H_2(0) \rightleftarrows HF(0) + H$	$9.0 \times 10^{12}\ \exp(-805/T)$
11	$HF(4) + H \rightleftarrows H_2(0) + F$	$1.0 \times 10^{12}\ T^{0.67}$
14	$H + F_2 \rightleftarrows HF(0) + F$	$6.0 \times 10^{12}\ \exp(-1208/T)$
21	$H_2(1) + M_1 \rightleftarrows H_2(0) + M_1$	$2.5 \times 10^{-4}\ T^{4.3}$
23	$HF(1) + M_3 \rightleftarrows HF(0) + M_3$	$9.0 \times 10^{8}\ T^{1.3}$
31	$HF(1) + M_6 \rightleftarrows HF(0) + M_6$	$5.0 \times 10^{7}\ T^{1.3} + 1.0 \times 10^{16}\ T^{-1.43}$
39	$HF(1) + M_5 \rightleftarrows HF(0) + M_5$	$1.3 \times 10^{-2}\ T^{3.6}$
47	$2HF(1) \rightleftarrows HF(0) + HF(2)$	$4.0 \times 10^{5}\ T^{2.2}$
54	$HF(1) + HF(2) \rightleftarrows HF(0) + HF(3)$	$1.3 \times 10^{3}\ T^{2.8}$
60	$HF(1) + HF(3) \rightleftarrows HF(0) + HF(4)$	$6.0 \times 10^{-2}\ T^{3.9}$

*Nominal values; Units: T in °K, time in sec, volume in cm^3, mass in moles.
The M_i's denote catalytic species

M_1 = H, F, Ar, HF(0), ..., HF(8)
M_2 = 20*H, F, Ar, HF(0), ..., HF(8), 2.5*H_2(0), 2.5*H_2(1), 2.5*H_2(2), F_2
M_3 = F.
M_4 = H, F, Ar, HF(0), ..., HF(8), H_2(0), H_2(1), H_2(2), F_2
M_5 = H, Ar, H_2(0), H_2(1), H_2(2), F_2
M_6 = HF(0), ..., HF(8)

Coefficients such as "20*" in the list of catalytic species denote that the species concentration is weighted by this factor in computing the reaction r ..

the rate coefficients were assumed to be undertain to within a multiplicative factor or 5, independent of temperature. At every temperature each rate coefficient k_i was assumed to have a uniform probability distribution of its logarithm within bounds given by

$$\log k_i^{(o)} - \log 5 \leq \log k_i \leq \log k_i + \log 5. \qquad (4.13)$$

where $k_i^{(o)}$ is the nominal value of k_i, i.e., the value tabulated in Table 4.7. We note in passing that for such a distribution, the transformation function G_i of Eq. (3.1) is given by

$$G_i(x) = \frac{2}{\pi} \mathrm{Sin}^{-1}(x) \ , \qquad (4.14)$$

where Sin^{-1} is the principal value of the inverse sine function.

The number of fluorine atoms produced at time t = 0 by flashlamp discharge is similarly uncertain by about a factor of two [15], i.e., for this parameter log 5 is replaced by log 2 in Eq. (4.13).

The differential equation system which describes the laser at zero power was programmed and run. Initial conditions of temperature and composition were as indicated in Table 4.8.

The laser model was integrated from zero time out to a real time of 4.0 microseconds. With fourteen parameters it was necessary to carry out 907 such integrations.* Data

*This is based on the rule $N = 2\omega_{max} - 7$ mentioned previously, in Section III and not on the rule $N = 2\omega_{max} + 1$.

TABLE 4.8

INITIAL CONDITIONS FOR LASER STUDY

Temperature 300°K

Species Concentrations

Ar (inert diluent)	4.704×10^{-5} mole cm^{-3}
$H_2(0)$	9.407×10^{-7} mole cm^{-3}
$H_2(1)$	1.119×10^{-15} mole cm^{-3}
$H_2(2)$	4.321×10^{-24} mole cm^{-3}
H	0.0 mole cm^{-3}
$HF(v')$ ($v' = 0$ to 8)	0.0 mole cm^{-3}
$F + 2F_2$	1.975×10^{-6} mole cm^{-3}
F (nominal value)*	4.704×10^{-8} mole cm^{-3}
F_2 (nominal value)**	1.928×10^{-6} mole cm^{-3}

* Actual initial value ranges from -50% to 100% of tabulated value (see text).

** Actual initial value dependent upon initial F atom concentration, such that sum $F + 2F_2$ is tabulated value.

on populations of vibrational states, chemical concentrations, temperature, and other variables was stored at each 100 nanosecond real time interval. From the populations N(v) of adjacent vibrational levels of HF, it is simple to calculate the gains. The gain $\alpha(v,J)$ for the transition HF(v+1, J-1) → HF(v,J) (J is the rotational quantum number of the lower vibrational state) is expressed by

$$\alpha(v,J) = \frac{hN_A}{4\pi}\,\omega_c(v,J)\,\phi(v,J)\,B(v,J)\left\{\frac{2J+1}{2J-1}\,N(v+1,J-1)-N(v,J)\right\} \tag{4.15}$$

where h is Planck's constant, N_A is Avogadro's number, ω_c is the wavenumber of the transition, $\phi(v,J)$ is the line profile at line center,* $B(v,J)$ is the Einstein coefficient for absorption, and N(v,J) is the population of the v,J rotation-vibration level of HF. The assumption of thermal equilibrium of the rotational states implies that N(v,J) satisfies

$$N(v,J) = N(v)\,(2J+1)\exp(-hcE_J^v/kT)/Q_r^v(T) \tag{4.16}$$

where k is Boltzmann's constant, T is the absolute temperature (assumed the same for rotation and translation), E_J^v is the rotational energy of the v,J level relative to the v,0 level, and $Q_r^v(T)$ is the rotational partition function:

$$Q_r^v(T) = \sum_J (2J+1)\exp(-hcE_J^v/kT). \tag{4.17}$$

In evaluating the gain as a function of time it is necessary to search over the rotational quantum number J to find that

*The Doppler profile was assumed in the model.

J value which maximizes $\alpha(v,J)$ as a function of time. The reason for this is that only one such level can lase at any given time within each vibrational band, and it is the level for which $\alpha(v,J)$ is maximum that actually lases. This J value can shift in time. The search procedure is simple and straightforward.

We will describe the results of the sensitivity analysis for the v = 2→1, v = 3→2, and v = 4→3 bands. The report by Levine [9] analyzed many other variables in addition to these three, and the reader can refer to this report for additional discussion. The three variables we will describe here suffice to illustrate the technique of application of sensitivity analysis.

Figure 4 shows the zero-power gain as a function of time for the v = 2→1, v = 3→2, and v = 4→3 transitions. Both the nominal values and the mean values (averaged over the distribution of all parameters) are shown. Except at times less than 1 μsec following initiation the mean and nominal values differ considerably, both for the v = 2→1 and v = 3→2 transition. For the v = 4→3 transition, the mean and nominal values are not in good agreement even at times as short as 0.2 μsec. From this we can infer that the variance of these transitions will be large, which is confirmed in Figure 5, where we plot the coefficients of variation. From these two figures we see that the predictive ability of the model is poor as a consequence of the parameter uncertainties.

The question as to which parameter uncertainties cause this high variance is answered graphically in Figures 6, 7, and 8. These three figures display the partial variances for the v = 2→1, v = 3→2, and v = 4→3 gains, respectively.*

Reference to Figure 6 shows that for the v = 2→1 transition the variance at early times is due mainly to uncertainties in the initial F atom concentration $[F]_0$ and the rate coefficient for process $F + H_2(0) \rightleftarrows HF(0) + H$. Since the coefficients for the process $F + H_2(0) \rightleftarrows HF(v) + H$ (v = 1, 2, 3) are proportional to this rate (c.f., References 9 and 14) this is equivalent to stating that calculation of the gain at early times is sensitive to the rates at which reaction of F with $H_2(0)$ populates the excited levels, as we should anticipate.

At longer times the sensitivity coefficient for the collisional deactivation process $HF(v) + HF(v') \rightleftarrows HF(v-1) + HF(v')$ becomes the dominant cause for uncertainty in the computed values of the gains. At still longer times the uncertainties in the rate coefficient for the process $H + F_2 \rightleftarrows HF(0) + F$, and in the initial concentration of F atoms, become the dominant sources of uncertainty. The reason for the importance of the latter parameter at late times is related to the fact that the laser at zero-power operates adiabatically.[9] The reason for the importance of the former parameter at late times is that the collection of reactions $H + F_2 \rightleftarrows HF(v) + F$ tends to

*The curves only show those partial variances which are large. Parameters whose partial variances are negligible are not shown, so as to avoid cluttering the figures.

repopulate the excited levels HF(v) ($v \geq 1$) following their initial depopulation. The rate coefficients for this process with $v \geq 1$ are taken to be proportional to the rate coefficient for this process with v = 0, c.f., References 9 and[13].

Reference to Figure 7 shows that the variance in the computed zero-power gain at the v = 3→2 transition is due to substantially the same reasons as in the case v = 2→1, with small additional influences. The latter correspond to the processes $HF(v) + H \rightleftarrows F + H_2(0)$ (v = 4, 5, 6) and $2HF(v) \rightleftarrows HF(v-1) + HF(v+1)$. The former process, while it does not directly involve the states HF(2) and HF(3), nonetheless influences these states indirectly, since, e.g., removal of molecules from HF(4) by collision with H eliminates molecules in HF(4) as a source of molecules in HF(3) via the process $HF(4) + HF(v) \rightleftarrows HF(3) + HF(v)$.

Reference to Figure 8 shows a feature unique to the zero-power gain on the v = 4→3 transition. The process $HF(v) + H \rightleftarrows H_2(0) + F$ (v = 4, 5, 6) is the dominant cause of variance in the computed gain at times beyond 1.0 μsec. Furthermore, as can be seen in Figure 5, the variance for the gain on this transition is larger than that for the other transitions. It is striking also to note that the computed gain on this transition is very small (see Figure 4), a fact which can be related to a very low population for the v = 4 level.[9,10] It thus becomes possible to suggest, as a consequence of the sensitivity analysis, that the

anomalously small computed gain on the v = 4→3 transition may be due to too large a nominal value for the rate coefficient of the process $HF(4) + H \rightleftarrows H_2(0) + F$. For further discussion of this point, we refer the reader to the report by Levine.[9]

In concluding this example, it is worth noting that the results of the sensitivity analysis show that the predictions of the model are sensitive only to five of the 14 parameters studied. Thus we find that the large uncertainties in the remaining nine parameters do not influence the predictions. In view of this, we can conclude that for all practical purposes those processes for which the sensitivity coefficient is small can be omitted from the model entirely. That is to say, a simplified five reaction model would suffice to describe the HF laser at zero power.

3. A SOCIOECONOMIC MODEL (WORLD II)

Forrester has written extensively on the use of mathematical models as descriptions of industrial and social processes.[16] World II[17] is an example of a model of this type. It consists of five coupled differential (or difference) equations* describing the time dependence of five variables: population, natural resources, capital investment, pollution, and the fraction of capital which is in agriculture. The model utilizes a large number of parametric relations to relate the time rates of change of the dependent variables to current values of these variables. Many of these relations consist of tabulations, so that each table entry constitutes a parameter. As such, the model contains several hundred parameters, each of which contains to some extent biases of the model's author. In any event, none of these parameters are precisely known, and these parametric

*Typically the models developed by Forrester consist of coupled difference equations in a set of dependent variables with time as independent variable. The change $x_n - x_{n-1}$ in a typical dependent variable over one time interval $\Delta t = n\Delta t - (n-1)\Delta t$ is usually expressed as a forward difference, i.e., $x_n - x_{n-1}$ is assumed to depend upon the set of dependent variables $\{x_{n-1}\}$, plus in some case independent driving functions, all evaluated at time $t = (n-1)\Delta t$. In the limit $\Delta t \to 0$ the system of equations would reduce to a system of ordinary differential equations. As compared to the differential equations so derived, Forrester's difference equations can be viewed as being the forward Euler difference approximation to the differential equation. As such, the possibility arises that the difference equations may be relatively unstable compared to the differential equations, and that, therefore, the difference form may generate solutions which depend sensitively upon the time step employed. To our knowledge, no specific stability analysis of Forrester's World II model has been performed, but the numerical solutions show no evidence of artificial mathematical instabilities induced by the difference scheme used.

uncertainties will influence the prediction of the model. We selected a small subset, nine in number, of the parameters and examined the sensitivity of the model to assigned uncertainties in these parameters. The parameters we studied are listed in Table 4.9, along with the "identifiers" used in the original study.

The first four parameters listed in Table 4.9 are annual rates of growth or decay. The last of these parameters, CIDN, basically is identical to the rate of depreciation of capital. The fifth parameter, "normal pollution", is a multiplier which gives the rate of generation of pollution per unit of population, the unit of pollution being given by definition in terms of a standard unit defined so that the per capita global pollution in 1970 is one unit.

The sixth parameter, BETA, is related to the rate of absorption of pollution, i.e., its conversion to harmless form, by the global ecosystem. Forrester assumes a quasilinear relation between absorption time and level of pollution (see Figure 3-15, p. 57, of Reference 17). For such a case, the rate of change of pollution p, would be given by

$$dp/dt = -p/\alpha(p) + \text{source terms} \qquad (4.19)$$

where the characteristic decay time α is itself a function of p. We have scaled Forrester's estimate of $\alpha(p)$ by a constant factor β, i.e., we use

$$dp/dt = -p/\beta\alpha(p) + \text{source terms}, \qquad (4.20)$$

TABLE 4.9

PARAMETERS OF WORLD II MODEL STUDIED BY SENSITIVITY ANALYSIS

	Identities	Description	Nominal Value
1.	BRN	Normal birth rate	0.04 $year^{-1}$
2.	DRN	Normal death rate	0.028 $year^{-1}$
3.	CIGN	Normal capital investment growth rate	0.05 $year^{-1}$
4.	CIDN	Normal capital investment decay rate	0.025 $year^{-1}$
5.	POLN	Normal pollution	1.0
6.	BETA*	Scale factor for pollution absorption time	1.0
7.	CIAFT	Capital fraction in agriculture	15.0 years
8.	C*	Coefficient of CFIFR in rate of charge of CIAF (see text)	1.0
9.	NRI	Initial inventory of natural resources	9.0×10^{11}

*Not defined in original World II model. See text for explanation.

and our sixth parameter is this scale factor β (BETA). Values of BETA in excess of unity correspond to ecosystem recovery slower than that assumed by Forrester; values of BETA less than unity correspond to ecosystem recovery faster than that assumed by Forrester.

The seventh parameter is a relaxation time which fixes the rate at which capital investment can be shifted into or out of agriculture in response to the variations in demand for agricultural capital (e.g., tractors, harvesting equipment), this demand also being dependent upon the instantaneous supply-demand relation for food.

The eighth parameter is similar in character to the sixth. Forrester assumes that the rate of change of the fraction of capital investment devoted to agriculture is related to the per capita food supply (see Figure 3.13, p. 59 of Reference 17), with larger food availability leading to decreasing rate of capital investment in agriculture, and vice versa. His assumed relation is roughly exponential, with <u>all</u> new capital invested in agriculture in the limit of zero food availability; with 30 percent of new capital devoted to agriculture when the per capita food availability (the "food ratio") is at a "satisfactory" level (unity by definition), and 9 percent of new capital when food supply is twice per capita need. We can express this relation as $f = \exp(-1.204\ r)$ where f is the capital fraction (CIAF) indicated by the food ratio (CFIFR) and r is the food ratio.

In our analysis, we generalize this relation to read $f = C\exp(-1.204r)$, so that values of C in excess of unity correspond to increasing the rate at which new capital is switched into agriculture in response to food shortages, as compared to the standard rate assumed by Forrester, and values of C less than unity correspond to decreasing this rate as compared to Forrester's assumption.*

The last parameter is the inventory of natural resources in the initial year of the model, in arbitrary resource units. The nominal value of this inventory is what is presumed available in the year 1900, with a per capita need of 1 unit/year. This supply then would suffice for 250 years for a (fixed) population of 3.6×10^9 individuals.

A major criticism of World II has been that its resource inventory is finite and irreplacable. In such a case this initial value must become the dominant parameter at sufficiently long times. Rather than try to introduce renewable resources, technological innovation, or other mitigating concepts, we have chosen to analyze World II as is. Therefore, we will inevitably be confronted with a world in which everyone dies in the long term. At issue, however, is the question of the reliability of World II on a relative basis in the intervening time.

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*At first sight it might appear that when C > 1 and the shortage of food is acute, the system will "try" to devote more than 100 percent of all new capital to agriculture. Needless to say, it cannot succeed in doing so, as careful analysis shows. But it does mean that net rate of response to "starvation" is better than in the standard case.

One auxiliary variable is important. Forrester defines a "quality-of-life" function as the product of four factors, each dependent upon one of the dependent variables: population, food, capital investment per capita (termed "material"), and pollution. There are several arbitrary aspects to his definition,* such that the numerical value is best viewed only as qualitative and not quantitative. Nonetheless, to lay stress on the difficulty of predicting qualify of life, we have treated this variable as quantitative, and have subjected its predicted values to sensitivity analysis.

We obtained a computer program for World II,** and applied our method. Except for the nine parameters listed in Table 4.9, all parameters were given the values used by Forrester for his "base case". For the nine parameters of Table 4.9, the nominal values, as given in the table, correspond to Forrester's base case. We attributed to each of

* We are tempted to suggest that a Delphi procedure might provide the most rational way of determining a consensus definition of quality-of-life.

** We are indebted to Professor W. E. Schiesser, Department of Chemical Engineering, Lehigh University, for supplying us with this program. This program uses second order forward Runge-Kutta integration instead of first order forward Euler differencing. It is possible to prove that this Runge-Kutta method has wider stability bounds than the forward Euler method, so that with equal or smaller time-steps than those used by Forrester, we are assured that our solutions display the same stability character as Forrester's original equations. We in fact used smaller time-steps, so that numerically we always generated solutions with the same stability characteristics as in the original work.

these nine parameters an uncertainty of ± 20 percent, with a uniform distribution of probability within this interval. In view of the difficulty in precisely ascertaining values for these parameters, it appears to us that attribution of a ± 20 percent error understates the real situation.

The output (dependent) variables we analyzed were population, pollution, capital investment, natural resources, and quality of life. In this paper we only discuss the first and last of these.

Figures 9 and 10 show our results for population. In Figure 9 we see that the nominal and mean values of population are virtually coincident until about Year 1976 (they also coincide fairly well with real data) but that beginning about Year 1976 a divergence sets in.* This divergence reaches an (absolute) maximum about Year 2040, at which time the mean value is about one billion (1×10^9) persons lower than the nominal value. The corresponding value of the coefficient of variation also is shown; it reaches a maximum value of about 0.4 in Year 2040.

The sensitivity coefficients for population are shown in Figure 10. The graph exhibits only four of the nine parameters because for the other five the coefficients are very

*We see here a remarkable example of the well-known fact that models do a better job of confirming the past than of predicting the future!

small, and effectively zero. It is interesting to note that in early years, i.e., pre 1930, the birth and death rates, which are direct influences of population, are the dominant parametric influence in population. However, at later times, the normal capital investment growth rate emerges as the most important parameter, and the variance in population prediction is dominated by the uncertainty in this investment rate.

The peculiar effect, near Year 2010, where nearly all of the sensitivity coefficients fall to zero arises from an inadequacy in our procedure as applied to this one example; at the time we did this calculation (mid 1974) we were not yet aware of the significance of the harmonics in the definition of the sensitivity coefficients, so that we were computing coefficients by calculating the fundamental terms of Eq. (2.25) only. In such a calculation, it is possible to "lose" some of the variance when the coefficient of the Fourier fundamental undergoes a change in sign (c.f., Section II for a discussion of this possibility). This circumstance applies for population in Year 2010. It would be interesting to repeat our calculation using the fuller definition, Eq. (2.25), but we have not had the opportunity to do so. Nonetheless, it seems clear to us that the uncertainty in the normal capital investment growth rate is the key parameter which leads to variance in the predicted population.

Figures 11 and 12 show our analysis of the auxiliary variable quality of life. In Figure 12 we see that the

mean and nominal values of this variable are virtually coincident until about Year 2005, but that following this year the mean value rises to a dramatic new level whereas the nominal value continues to decay. After about Year 2045 the mean value rapidly decays. The coefficient of variation is small until Year 2005, but then rises dramatically over the next 15 years, following which it too decays. The long term decay (i.e., after Year 2050) of the mean and nominal values and the coefficient of variation all are traceable to the finite resource inventory in the model. The influence of the latter only is beginning to appear at about Year 2070, but is clear enough that with an inventory capable of sustaining 3.6×10^9 people for 250 years, and populations as exhibited in Figure 9, depletion of resources is going to be of overriding significance in the model by Year 2150 = 1900 + 250, i.e., just off the figure at the right.

It is striking to see that the model is more likely to lead to a prediction of a "golden age" in the period 2005-2050 than it is to predict a continuing decay, if an accounting is made of parameter uncertainties.

Figure 12 shows the sensitivity coefficients for the quality of life: birth and death rate are the important parameters prior to 2005; however, since the variance is small in these years, it is not too significant to inquire as to the causes of the variance. After Year 2020, the normal capital investment growth rate becomes the most

important single parameter, although it by no means dominates quality of life to the degree it dominates population. Still later in time, there is a transient period of importance for the normal capital investment decay rate, presumably due to the fact that with diminishing resources and hence limited capability for new capital formation, it is the rate of disappearance of capital to which quality of life is most sensitive.

To summarize then, the conclusions we have reached in our brief study of Forrester's model are:

1. Uncertainties as to the nominal rate of capital investment is the dominant parameter which renders predictions of World II unreliable, at least over the next 100 years.
2. To the extent to which the resource inventory is truly finite, the initial extent of this resource ultimately becomes the key parameter at some future point in time.
3. The model is not capable of predicting "quality of life" to any meaningful degree after about Year 2005.

More recently, Meadows et al.[18] have developed World 3, an extended and enlarged version of World 2, with many more variables, parameters, and equations. They subject this model to a number of linear sensitivity analyses, on the basis of which they determine the model's qualitative reliability. A much more appropriate test of the model's reliability would be via a nonlinear method such as the one discussed in this paper.

4. A CHEMICAL REACTION MODEL

In a recent paper[19], Boni and Penner have successfully applied our method of sensitivity analysis to a study of methane oxidation kinetics. Their model consisted of a set of 23 coupled rate equations involving 23 parameters, i.e. rate coefficients. These parameters were varied over a ±50% range of uncertainties about their nominal values $k_i^{(o)}$. The output functions were the species concentrations [CH_4, CH_3, CH_2O, CHO, CO, CO_2, H_2O, O, H, OH] at different times [10^{-7} to 10^{-2} seconds] after the initiation of the reaction. Their analysis showed "that of the 23 reactions, plus their inverses, included in the mechanism, only about 5-7 reactions (depending upon the species in question) strongly affect the concentration of that species". Their analysis thus provides an important example of how sensitivity analysis can be used to simply complex models by segregating the "important" and "unimportant" component equations.

V. Additional Research

There are a number of interesting and important problems which have arisen during the course of this research and to which we have not had an opportunity to address ourselves. We list them here briefly and hope that some of the readers of this review and future practioners of this method will be stimulated to carry out some work along these lines.

a) Postponement of Interferences:

In sections 2E and 2F above and in Appendix I, we have discussed the problem of interference which arises from the unavoidable use of a set of integer or rational frequencies. This effect can be "postponed" in the sense that we can chose a high value of M (see Eq. A1.4), the order of interference. As pointed out in refs. (1) through (3), however, the larger the chosen value of M, the larger the maximum value ω_{max} of the input frequencies set $\{\omega\}$ and correspondingly, the larger the number N of s-space points required for the evaluation of the Fourier amplitude. Thus, a large value of M, which will minimize the interferences, will appreciably increase the number of computations required for the calculation of the Fourier amplitudes. As we have shown, for instance, in ref. (3), 806 points in s-space are required for the calculation of the Fourier amplitudes $B\omega_{\ell}$ for a 10 parameter system for M=4, while 8,520 points are required for the same system when M=6.* Since ω_{max} will of course increase with the number n of parameters k_i, i=1,2,...,n, this problem becomes particularly serious for systems with a large number of parameters.

One obvious way to circumvent this problem completely would be to use a set of incommensurate frequencies $\underline{\omega}$. Since this does not seem a feasible on a computer with a finite register, the next best solution would be to

*Owing to the symmetry properties of f's) discussed in Section (3.2), the number of sample points required are only one-half of those listed here.

learn how to construct integer frequency sets $\{\omega\}$ which will lead to large values of M for reasonable values of ω_{max}. It is not clear how much of an improvement can be achieved on the frequency sets already published in our papers[1,2,3], but research along these lines is clearly desirable.

In this connection, attention should be called to our brief discussion in section 2F (see Eq. 2.20) on the spacing of the N quadrature points used in the calculation of the Fourier coefficients. It may well be possible to increase the accuracy of the computed Fourier coefficients by a more judicious choice of spacing which takes account of the oscillatory properties of the output function f(s). Some work on this problem could be very useful.

b) Expansion of Output Function $\underline{f}$

We have chosen in the work done so far to transform the output functions, $\underline{f}$ into periodic functions on $(0, 2\pi)$, see Eq. (2.7), and then Fourier analyse these functions to obtain their Fourier coefficients. Interestingly, there is nothing sacrosanct in expanding $\underline{f}$ in terms of sine and cosine functions. One could equally well expand $f(u)$, the output function in $\underline{u}$-space, in terms of any other desired or useful set of orthogonal functions, such as, for instance, Hermite polynomials. One would then have to establish again the connection between the expansion coefficients and some "sensitivity measure" as has been done above. It is not clear whether such expansions in terms of other orthogonal functions would lead to a simpler or better (or worse) theory of nonlinear sensitivity analysis, but it raises a question which could usefully be pursued.

c) Information in Harmonics and Combination Frequencies

As discussed in the previous sections, the Fourier spectrum of the output function contains harmonics and linear combinations of all the input frequencies ω_ℓ, $\ell = 1,2,\ldots,n$. In our earlier version of sensitivity analysis,

references (1) through (3), we have used only the information contained in the fundamentals ω_ℓ through the Fourier amplitudes B_{ω_ℓ}, Eq. (2.30). In the partial variance method outlined in section b above we have made use also of the harmonics of the fundamental frequencies for the construction of S_{ω_ℓ} as in Eq. (2.26). As pointed out in that section, Eqs. (2.27) through (2.29), it is also possible to construct higher partial variances $S^2_{\omega_\ell,\omega_k}$, $S^2_{\omega_\ell,\omega_k,\omega_j}$, etc. corresponding to linear combinations of the fundamental frequencies ω_ℓ, ω_k, ω_j, etc. These higher partial variances contain increasingly more detailed information about the coupling of sensitivity due to uncertainties of groups of parameters. Such information is clearly of great importance in studying the sensitivity of chemical and other complex rate systems since the explicit rate laws for the output functions, if they could be obtained, would most probably involve sums and products of various parameters. It would therefore be most useful to explore the construction of higher partial variances and analyze the information obtained from them in future applications of the Fourier method of sensitivity analysis.

d) Correlated Parameters

In all the work described so far we have made the explicit assumption that the system parameters k_ℓ and their variation u_ℓ over any desired range are uncorrelated. By this we mean that each parameter can be varied independently of all other parameter or, equivalently, that to each parameter one can assign a range of uncertainty with its probability distribution independent of the uncertainty range assigned to all other parameters. This is certainly valid for many physical systems where the parameters are indeed independent of one another and can be determined, theoretically or experimentally, independently of one another.

In many economic and social model systems there are, however, correlations betewen the parameters. Frequently it is not even possible to define parameters which are independent. The determinations of parameters in such systems by fitting models to repeated observations leads to a set of parameters which are statistically dependent, i.e. the range of uncertainty of parameter k_i may well be correlated with the uncertainty range of parameters k_j, k_ℓ, etc.

To take proper account of such correlated parameters one needs to modify the Fourier amplitude sensitivity method analysis. One way of doing this is to incorporate the concept of correlated parameters into the formulation of the sensitivity analysis theory from the outset. This means that one can not use the ansatz (2.3) according to which the probability density $P(\underline{u})$ is written as the product of the $P(u_i)$. We have not pursued this approach, and it is not clear what forms our theory will take when this simplifying assumption does not hold. Research on this problem is clearly of interest, particularly for the application of this method of sensitivity analysis to economic model systems.

Appendix I

The error ε in approximating an integral over $\underline{\theta}$-space by a line integral over the search curve, for the Fourier coefficients of frequencies $p\omega_\ell (p=1,2,\ldots)$ is represented by the difference

$$\langle f(s)e^{ip\omega_\ell s}\rangle - \langle f(\underline{\theta})e^{ip\theta_\ell}\rangle = \varepsilon\langle f(\underline{\theta})e^{ip\theta_\ell}\rangle \quad . \tag{A1.1}$$

Here, ε is given by the sum

$$\varepsilon = \sum_{\underline{r}}{}' \; c_{\underline{r}}\, \delta(\underline{r}\cdot\underline{\omega} - p_\ell\omega_\ell) \tag{A1.2}$$

wnere the prime on the summation excludes the $c_{0\ldots p_\ell \ldots 0}$ term, i.e., the $r_1 = r_2 = \ldots = r_{\ell-1} = r_{\ell+1} = \ldots r_n = 0, r_\ell = p_\ell$ Fourier coefficient. The Kronecker delta is defined as

$$\delta(\underline{r}\cdot\omega) = \left.\begin{array}{ll} 1 & \text{for } \underline{r}\cdot\omega = 0 \\ 0 & \text{for } r\cdot\omega \neq 0 \end{array}\right\} \tag{A1.3}$$

This result is obtained by using the definition, Eq. (2.14), of $f(\underline{\theta})$ as a multiple Fourier series in the θ_i's in Eq. (A1.1). As can be seen from Eq. (A1.2), each time $\underline{r}\cdot\underline{\omega} = p_\ell\omega_\ell$, one obtains a contribution to the error ε made in equating the s and $\underline{\theta}$ space integrations. We refer to the values of $\underline{r}$ which satisfy $\sum_i r_i\omega_i = p_\ell\omega_\ell$ as <u>interferences</u>. The weight of the error is just the Fourier coefficient $c_{\underline{r}}$ evaluated at the value of $\underline{r}$ for which $\underline{r}\cdot\underline{\omega} = p_\ell\omega_\ell$. Since Fourier coefficients tend to decrease in magnitude as their index $\underline{r}$ increases, we see that postponing the occurrence of interferences to higher values of r will lead to a smaller error ε.

It is convenient to define M_1, the order of an interference such that $\underline{r}\cdot\underline{\omega} \neq p_\ell \omega_\ell$ for

$$\sum_{i=1}^{n} |r_i| \leq M_1 + p_\ell \quad . \tag{A1.4}$$

The higher the order of interference, the smaller the error ϵ for a given output function.

The values of $\underline{p}$ which lead to interferences are controlled by the choice of frequencies $\underline{\omega}$. Thus, a "judicious" choice of $\underline{\omega}$ leads to error terms which are small. By way of illustration we return to the two dimensional frequency choices given in Eqs. (2.12). Let us say that we are interested in the Fourier coefficient $C_{2\omega_1}$ and thus $p_\ell = 2$. For the first choice ($\omega_1 = 1$, $\omega_2 = 2$), the lowest interference arises when say $p_1 = 2$, $p_2 = -1$ so, with reference to Eq. (A1.4), $M_1 = 1$. This choice of frequencies leads to a poor coverage of $\underline{\theta}$ space and therefore a large error in equating s and $\underline{\theta}$ space integrals. The second frequency choice, $\omega_1 = 11$ $\omega_2 = 13$, leads to an interference when $p_1 = 13$ and $p_2 = -11$ so that $M_1 = 22$. The $\underline{\theta}$-space coverage is much improved and we obtain a more accurate value for the $\underline{\theta}$-space integration. By choosing frequencies which are increasingly incommensurate as measured by an increasing value of the order of interference one has, as $M_1 \to \infty$, the strict equality of s and θ space integration.

Appendix II

The results of Appendix I must be modified to account for the use of a finite number of points N that are used to carry out the s-space integration. The difference between the s-space quadrature and the $\underline{\theta}$-space average can be written as

$$C^*_{p\omega_\ell} - C_{p_\ell} = \varepsilon^* C_{p_\ell} \tag{A2.1}$$

where here ε^* is found to be (see ref. 3)

$$\varepsilon^* = \sum_{j=-\infty}^{+\infty} {\sum_{\underline{r}}}' C_{\underline{r}} \, \delta(\underline{r}\cdot\underline{\omega} - p_\ell\omega_\ell - jN) \quad . \tag{A2.2}$$

As in Eq. (A1.2), the prime on the summation excludes the coefficient $C_{\underline{r}} = C_{p_\ell}$ from the summations over r_i $(i = 1,2,\ldots,n)$. The error ε^* now includes contributions when $\underline{r}$ satisfies

$$\underline{r}\cdot\underline{\omega} - p_{\ell-\ell} = jN \; ; \quad j = \pm 1, \; \pm 2, \; \ldots \quad . \tag{A2.3}$$

That is, in addition to the interference errors (those arising for j=0), each time an integer multiple of N, the number of points in the quadrature, equals the frequency $\underline{r}\cdot\underline{\omega} - p_\ell\omega_\ell$, an additional error, whose size is given by the θ-space Fourier coefficient of that frequency, also occurs. We term these contributions to the error as aliases. The aliasing phenomena, which arise from the finite number of points used to numerically evaluate the Fourier coefficients, can also be controlled by appropriate choice of $\underline{\omega}$ and N. Postponing the aliasing to values of $C_{\underline{r}}$ with $\underline{r}$ larger and larger will yield a more accurate Fourier coefficient approximant $C^*_{p\omega_\ell}$. As for interferences, we define the order of an alias M_2 such that $\underline{r}\cdot\underline{\omega} \neq p_\ell\omega_\ell + jN$ $(j = \pm 1, \pm 2, \ldots)$ for

$$\sum_{i=1}^{n} |r_i| \leq M_2 + p_\ell . \qquad \text{(A2.4)}$$

Postponing the occurrence of aliasing by appropriate choices of $\underline{\omega}$ and N which lead to a large value of M decreases the error due to aliasing. For further details see ref. (3).

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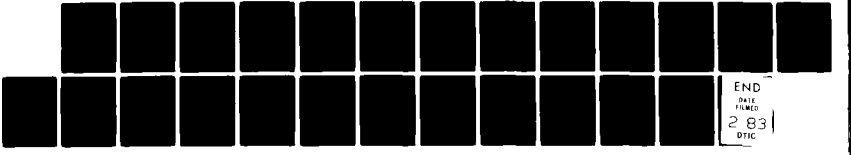

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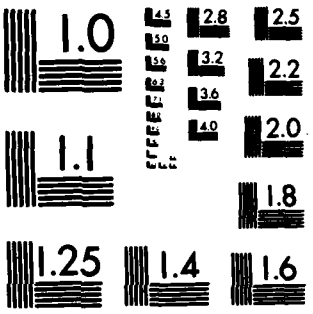

Appendix III

In the numerical computation of the Fourier coefficients, an N point approximation to the $\underline{u}$-space integration is used. In order to assess our approximations, we have constructed upper bounds on the error made for given $\underline{\omega}$,N sets and classes of output functions to be analyzed. We have described this error analysis in some detail in ref. (3) and will only sketch here its features and adopt them to the new approach to sensitivity analysis developed in this work.

The error made in the numerical evaluation of the Fourier coefficients is just the difference between the N-point quadrature formula and the integral over all $\underline{u}$-space. For, if we could use a space filling search curve in $\underline{u}$-space, Weyl's theorem would be exact and the Fourier coefficient evaluation would be exact. Thus, we define the error Δ_ℓ as

$$\Delta_\ell = \left| \left(\frac{1}{2\pi}\right)^n \int d\underline{\theta}\, g_\ell(\underline{\theta}) - \frac{1}{N} \sum_{q=1}^{N} g_\ell(\underline{\theta}_q) \right| \Big/ \left| \left(\frac{1}{2\pi}\right)^n \int d\underline{\theta} g_\ell(\underline{\theta}) \right| \qquad \text{(A3.1)}$$

where $g_\ell(\underline{\theta}) = f(\underline{\theta})e^{i\theta_\ell}$, $\underline{\theta}_q \equiv (\theta_{1q}, \theta_{2q}, \ldots, \theta_{nq})$ and $\theta_{jq} = \omega_j s_q$ with $j = 1,2,\ldots n$. We now construct an upper bound Δ_ℓ^{sup} to the error Δ_ℓ which is a function of $\underline{\omega}$,N and the output function to be evaluated. Note that $g_\ell(\underline{\theta})$ is multiply periodic in $\underline{\theta}$, and if the partial derivatives

$$\frac{\partial^{p^\ddagger} g_\ell(\underline{\theta})}{\partial\theta_1^{p_1}\partial\theta_2^{p_2}\ldots\partial\theta_n^{p_n}}; \qquad 0<p^\ddagger\leq p-1;\ 0<p_j\leq p-1;\ \sum_{j=1}^{n} p_j = p^\ddagger \qquad \text{(A3.2)}$$

are of bounded variation, then the Fourier coefficients $b_{\underline{r}}$ of $g_\ell(\underline{\theta})$

defined by

$$g(\underline{\theta}) = \sum_{\underline{r}} b_{\underline{r}} e^{i\underline{r}\cdot\underline{\theta}} \tag{A3.3}$$

satisfy

$$b_{\underline{r}} \leq \alpha_p \left| \prod_{j=1}^{r} r_j^{\ddagger} \right|^{-p} \tag{A3.4}$$

with α_p independent of $\underline{r}$ and $r_j^{\ddagger} = \max(1,|r_j|)$. The equality of Eq. (A3.4) provides the Fourier coefficients $b_{\underline{r}}^{sup}$ for the construction of Δ^{sup}. That is, since $g_\ell(\underline{\theta})$ is multiply periodic in $\underline{\theta}$, we use its multiple Fourier expansion in Δ_ℓ and obtain

$$\Delta_\ell \leq \Delta_\ell^{sup} \tag{A3.5}$$

with

$$\Delta_\ell^{sup} = \sum_{\underline{r}}' \sum_{j=-\infty}^{+\infty} b_{\underline{r}}^{sup} \delta(\underline{r}\cdot\underline{\omega}-j\Pi). \tag{A3.6}$$

One can readily construct the function $g^{sup}(\underline{\theta})$ whose Fourier coefficients are $b_{\underline{r}}^{sup}$ and, with Eq. (A3.1), find Δ_ℓ^{sup} in terms of $\underline{\omega}$,N and the properties of the output functions to be considered. The description of the output function is given by the boundedness of its partial derivatives as described by the value of $p^{\ddagger}$ in Eq. (A3.2). In this fashion we have in reference (3) constructed bounds on the error for sets of $\underline{\omega}$,N which we have used in numerical calculations. The most important conclusion to be drawn from the error analysis presented in reference (3) is that the Fourier coefficients can be calculated with good accuracy by judicious choice of N and the frequency set $\underline{\omega}$ and that comparison of Fourier coefficients with a "safety factor" of about one order of magnitude yield valid sensitivity measures.

The bounds on the Fourier coefficients can readily be combined to yield bounds on the partial variances S_{ω_ℓ}. Thus, the Fourier coefficient analysis is directly applicable to the partial variances. It is important to note that as one examines the Fourier coefficients of higher harmonics of a fundamental, the accuracy with which they are approximated degenerates since one is using the same number and placement of points in a quadrature formula involving a function which is increasingly more oscillatory. However, the s-space Fourier coefficients themselves fall off in magnitude as one works with higher frequencies so that the Fourier coefficients for the higher frequencies do not have to be as precisely approximated as those for the lower frequencies.

Appendix IV

The part of the total variance σ^2 arising from the uncertainty of the ℓ'th parameter, when the output function is averaged over the uncertainties in all other parameters, is found by first integrating over all parameter uncertainties except for the ℓ'th. This integration is best done in $\underline{\theta}$ space where one may use the multiple Fourier decomposition of Eq. (2.14). Thus

$$f(\theta_\ell) = \int d\theta_1 \ldots d\theta_{\ell-1} d\theta_{\ell+1} \ldots d\theta_n f(\theta_1, \ldots \theta_n)$$
$$= \sum_{p_\ell} c_{00\ldots p_\ell \ldots 00} \exp[i p_\ell \theta_\ell]. \tag{A4.1}$$

Now form the variance σ_ℓ^2 of $f(\theta_\ell)$ with respect to the uncertainty in k_ℓ

$$\sigma_\ell^2 \equiv \int f^2(\theta_\ell) d\theta_\ell - [\int f(\theta_\ell) d\theta_\ell]^2 \tag{A4.2}$$
$$= \sum_{p_\ell=-\infty}^{+\infty} |c_{00\ldots p_\ell \ldots 00}|^2 .$$

We have found before (cf. Eq. (2.18)) that the $\underline{\theta}$-space Fourier coefficient $c_{00\ldots p_\ell \ldots 00}$ equals the s-space coefficient $C_{p\omega_\ell}$ so that σ_ℓ^2 can also be written as

$$\sigma_\ell^2 = \sum_{p=-\infty}^{+\infty}{}' |C_{p\omega_\ell}|^2 . \tag{A4.3}$$

As before, we must modify this result to correspond to the finite summations. We define σ_ℓ^{2*} to be

$$\sigma_\ell^{2*} = \sum_{p=-(N/2-1)}^{N/2}{}' |C^*_{p\omega_\ell}|^2 = \frac{1}{2} \sum_{p=1}^{N/2} (A^*_{p\omega_\ell} + B^{*2}_{p\omega_\ell}) + \frac{1}{4} A^{*2}_{N/2}.$$

Now form the quotient σ_{ℓ}^{2*} arising from the ℓ'th parameter and the total variance σ^{*2} and call it $S_{\omega_\ell}^*$, the <u>partial variance</u>

$$S_{\omega_\ell}^* = \frac{\sum_{p=-(N/2-1)}^{N/2} |C_{p\omega_\ell}^*|^2}{\sum_{j=-(N/2-1)}^{N/2} |C_j^*|^2} \quad . \tag{A4.5}$$

This result is Eq. (2.25) of the text.

Appendix V

We wish to establish the symmetry relations

$$f(\pi/2 + s) = f(\pi/2 - s) \tag{A5.1}$$

$$f(-\pi/2 - s) = f(-\pi/2 + s) \tag{A5.2}$$

of the output function f(s) for $-\pi/2 \le s \le \pi/2$ and to see how these relations reduce the size of the discrete samples along the closed search curve.

To do so, we stipulate that the ω_i's are <u>odd</u> integers and set $\omega_i = 2k + 1$. Thus

$$\sin[(2k+1)] = \sin[(2k+1)(\pi-s)] = -\sin[(2k+1)(\pi+s)] = -\sin[(2k+1)(2\pi-s)]. \tag{A5.3}$$

Applying these identities to all the parameters, we establish

$$f(\pi-s) = f(\sin\omega_1(\pi-s), \sin\omega_2(\pi-s), \ldots)$$

$$= f(\sin\omega_1 s, \sin\omega_2 s, \ldots) = f(s) \tag{A5.4}$$

and

$$f(\pi+s) = f(-\sin\omega_1 s, -\sin\omega_2 s, \ldots) = f(2\pi-s) \quad . \tag{A5.5}$$

Since $f(s) = f(s+2\pi)$ by construction, eq. (A5.5) also implies

$$f(-\pi+s) = f(s) \tag{A5.6}$$

Equation (A5.4) states that f(s) in the quadrant $\pi/2 \le s \le \pi$ is the mirror image about $\pi/2$ of f(s) in the quadrant $0 \le s \le \pi/2$; eq. (A5.6) states that f(s) in the quadrant $-\pi \le s \le \pi/2$ is the mirror image about $-\pi/2$ of f(s) in the quadrant $-\pi/2 \le s \le 0$.

Thus we need only evaluate f(s) in the range $=\pi/2 \le f(s) \le \pi/2$. This reduces the computational load by a factor of two relative to what was stated in references (1) through (3).

Appendix VI

The working equations of our sensitivity method yield the Fourier coefficients of Eqs. (3.13). Here we show how to obtain these equations by use of the symmetries of the output functions f(s) in s, Eqs. (3.8), and the symmetries of the trigonometric functions.

The Fourier coefficients

$$A_j^* = \frac{1}{r} \sum_{q=1}^{2r} f_q \cos js_q$$
$$B_j^* = \frac{1}{r} \sum_{q=1}^{2r} f_q \sin js_q \qquad \text{(A6.1)}$$

can be written, using these symmetries, as sums over the half interval $\pi/2 \le s_q \le \pi/2$

$$A_j^* = \frac{1}{r} \sum_{q=-(r-1)/2}^{0} [\cos js_q + \cos js_{-r-q}] f_q + \frac{1}{r} \sum_{q=1}^{(r-1)/2} [\cos js_q + \cos js_{r-q}] f_q \qquad \text{(A6.2)}$$

$$B_j^* = \frac{1}{r} \sum_{q=-(r-1)/2}^{0} [\sin js_q + \sin js_{-r-q}] f_q + \frac{1}{r} \sum_{q=1}^{(r+1)/2} [\sin js_q + \sin js_{r-q}] f_q \qquad \text{(A6.3)}$$

where we now define $s_q \equiv \pi q/r$ and set $f(s_q) = f_q$.

Application of the addition theorems for trigonometric functions allows us to rewrite eqs. (A6.2) and (A6.3) as

$$A_j^* = \frac{1}{r} [1 + (-1)^j] f_o + \sum_{q=1}^{(r-1)/2} [f_j + f_{-j}] \cos \frac{\pi jq}{r} \qquad \text{(A6.4)}$$

$$B_j^* = \frac{1}{r}[1 - (-1)^j] \sum_{q=1}^{(r-1)/2} [f_j - f_{-j}] \sin\frac{\pi jq}{r} . \qquad \text{(A6.5)}$$

Recalling that $r \equiv 2q+1$ we obtain the equations (3.13) given in section 3.

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11) G. Emanuel, N. Cohen, and T. A. Jacobs, "Theoretical Performance of an HF Chemical CW Laser," Aerospace Corporation Report No. TR-0172(2776)-2, February 1972; available from National Technical Information Service, 5285 Port Royal Road, Springfield, Virginia 22151, as Document No. AD-746685.

References Con't.

12) S. N. Suchard, R. L. Kerber, G. Emanuel, and J. S. Whittier, J. Chem. Phys. 57, 5066, 1972.

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14) N. Cohen, private communication.

15) G. Emanuel, private communication.

16) See, e.g., J. W. Forrester, Industrial Dynamics, MIT Press, Cambridge, Mass., 1961; J. W. Forrester, Urban Dynamics, MIT Press, Cambridge, Mass., 1969.

17) J. W. Forrester, World Dynamics, Wright-Allen Press, Inc., Cambridge, Mass., 1971.

18) D. L. Meadows, et al, Dynamics of Growth in a Finite World, Wright-Allen Press, Inc., Cambridge, Mass., 1974.

19) A. A. Boni and R. C. Penner, Combustion Science and Technology, 15, 99(1976).

Figure Captions

Figure 1: Definition of Terms for Simulation Models.

Figure 2: $\underline{\theta}$-space coverage with frequencies $\omega_1 = 1$, $\omega_2 = 2$ and 100 quadrature points N. The lines are obtained from $\theta_\ell = \omega_\ell s (\text{mod } 2\pi)$ $0 \leq s \leq 2\pi$ and the points from $\theta_{\ell q} = \omega_\ell s_q (\text{mod } 2\pi)$ with $s_q = 2\pi q/N$; $q = 1,2,\ldots N$.

Figure 3: θ-space coverage with $\omega_1 = 11$, $\omega_2 = 13$ and $N = 100$ computed in the same fashion as in Figure 1.

Figure 4: Zero power gains versus time for the $v = 2 \rightarrow 1$, $v = 3 \rightarrow 2$, and $v = 4 \rightarrow 3$ vibrational transitions of HF. Curves show the time histories for both the nominal parameter values and for the statistical mean value (average over the parameter uncertainties).

Figure 5: Coefficients of variation of the gains on $v = 2 \rightarrow 1$, $v = 3 \rightarrow 2$, and $v = 4 \rightarrow 3$ vibrational transitions of HF, as functions of time.

Figure 6: Partial variances for the zero power gain of the $v = 2 \rightarrow 1$ band of HF. Curves are labeled by the rate coefficients to which they correspond; $[F]_0$ curve is partial variance due to uncertainty in initial F atom concentration.

Figure 7: Partial variances for the zero power gain of the $v = 3 \rightarrow 2$ band of HF. Curves are labeled by the rate coefficients to which they correspond; $[F]_0$ curve is partial variance due to uncertainty in initial F atom concentration.

Figure 8: Partial variances for the zero power gain of the $v = 4 \rightarrow 3$ band of HF. Curves are labeled by the rate coefficient to which they correspond; $[F]_0$ curve is partial variance due to uncertainty in initial F atom concentration.

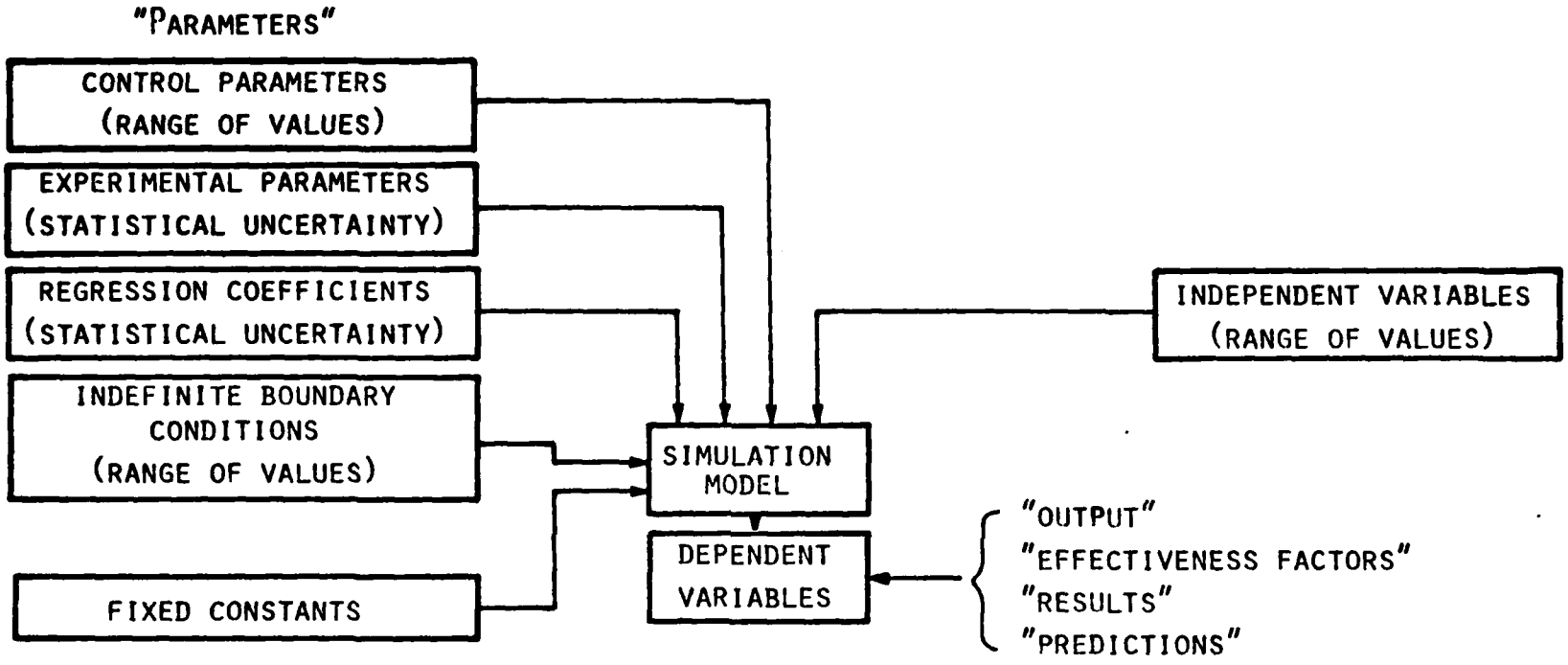
Figure 9: World population versus time.

Figure 10: Partial variances for world population. Curves are labeled by parameters to which they correspond. Three parameters, POLN, BETA and C have neglibible partial variances prior to 2020. After that time they have partial variances about equal to those for BRN and DRN. They are omitted from the figure so as not to complicate it. Other parameters have negligible partial variances.

Figure 11: Quality of life versus time.

Figure 12: Partial variances of quality of life. Curves are labeled by the parameters to which they correspond. The parameters POLN, BETA, and NRI have partial variances similar to CIDN. These are not shown in the figure to avoid confusion. Other parameters have negligible partial variances.

Fig. 1



INDEPENDENT VARIABLES:

CHANGE DURING THE COURSE OF A SINGLE RUN OF THE MODEL.

PARAMETERS:

DO NOT CHANGE DURING THE COURSE OF A SINGLE RUN OF THE MODEL.

DO CHANGE FROM RUN TO RUN OF THE MODEL.

FIXED CONSTANTS:

DO NOT CHANGE DURING THE COURSE OF A SINGLE RUN OF THE MODEL.

DO NOT CHANGE FROM RUN TO RUN OF THE MODEL.

Fig. 2

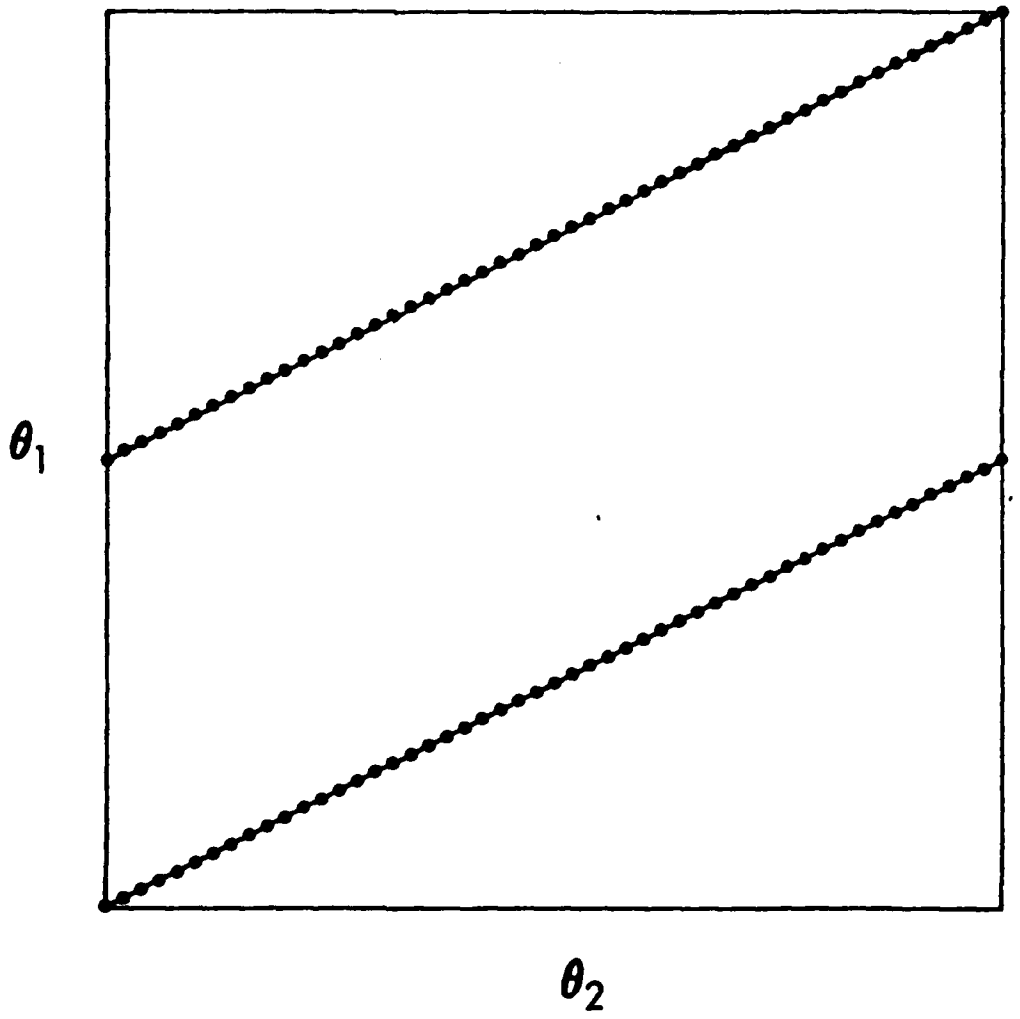


Fig 3

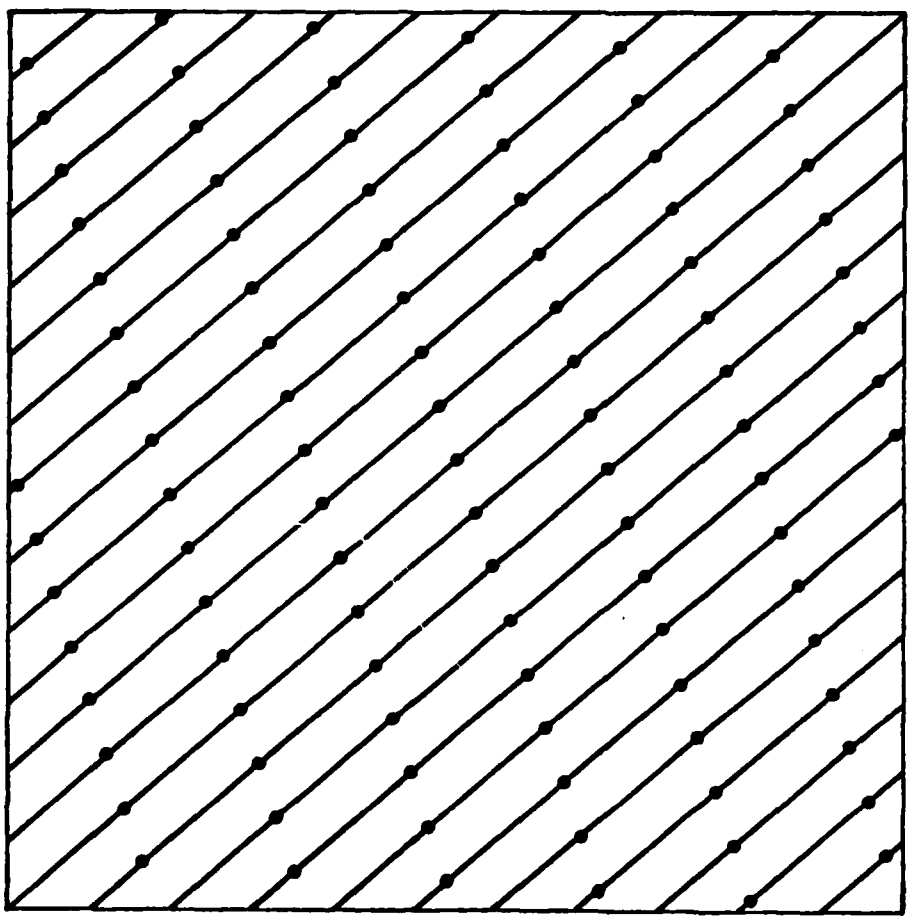


Fig. 4

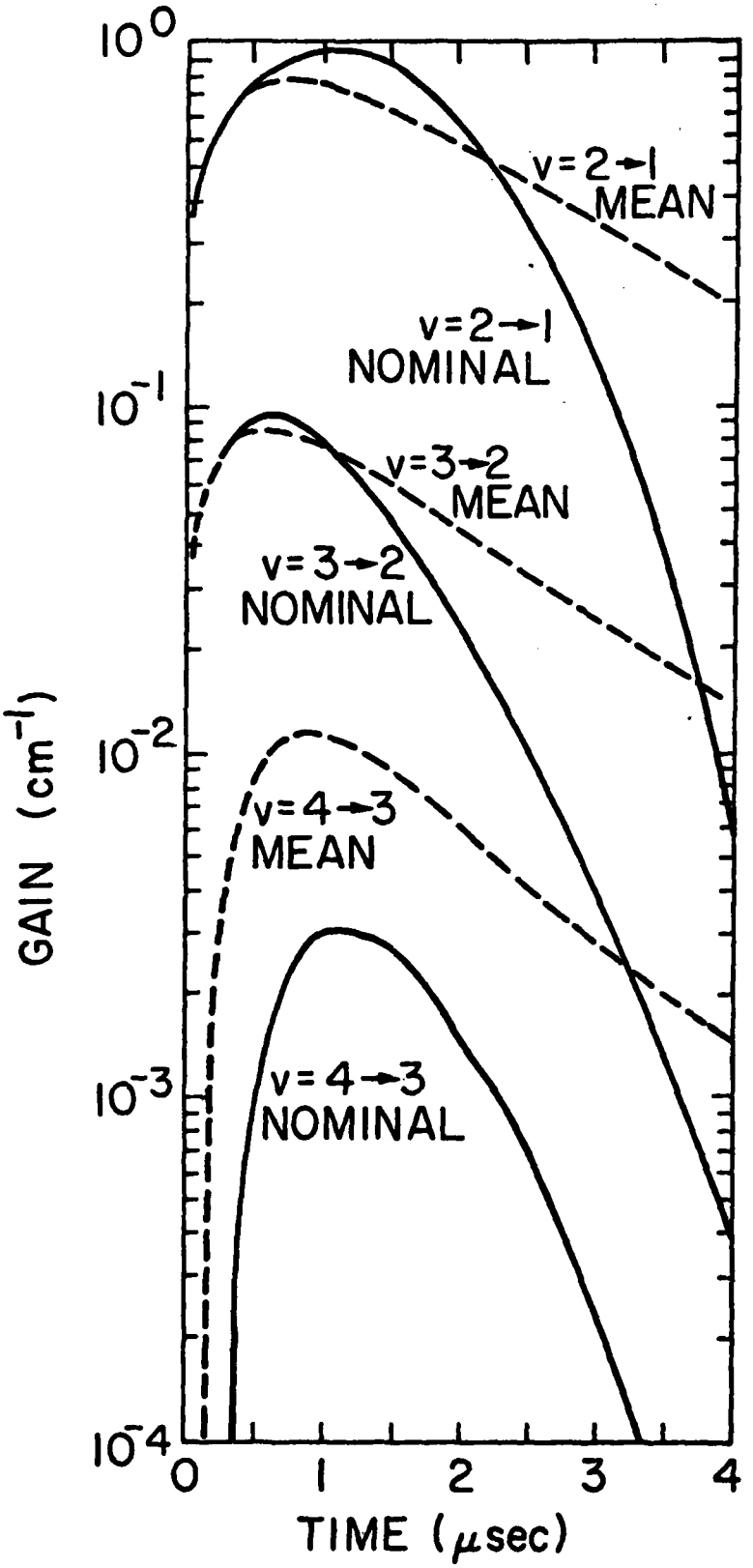

10^0
10^{-1}
10^{-2}
10^{-3}
10^{-4}
GAIN (cm^{-1})
v=2→1 MEAN
v=2→1 NOMINAL
v=3→2 MEAN
v=3→2 NOMINAL
v=4→3 MEAN
v=4→3 NOMINAL
0
1
2
3
4
TIME (μsec)

Fig. 5

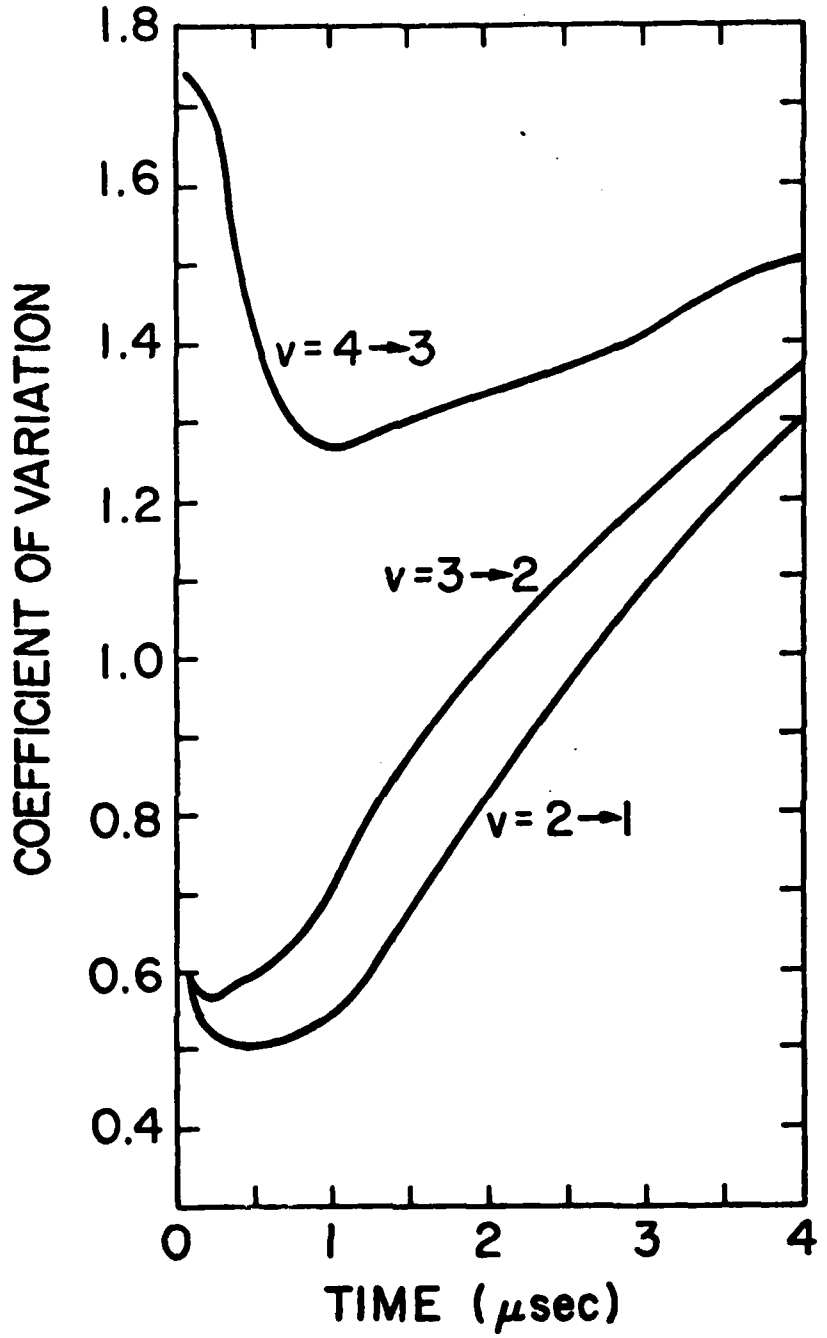

1.8
1.6
1.4
1.2
1.0
0.8
0.6
0.4
COEFFICIENT OF VARIATION
v=4→3
v=3→2
v=2→1
0
1
2
3
4
TIME (μsec)

Fig. 6

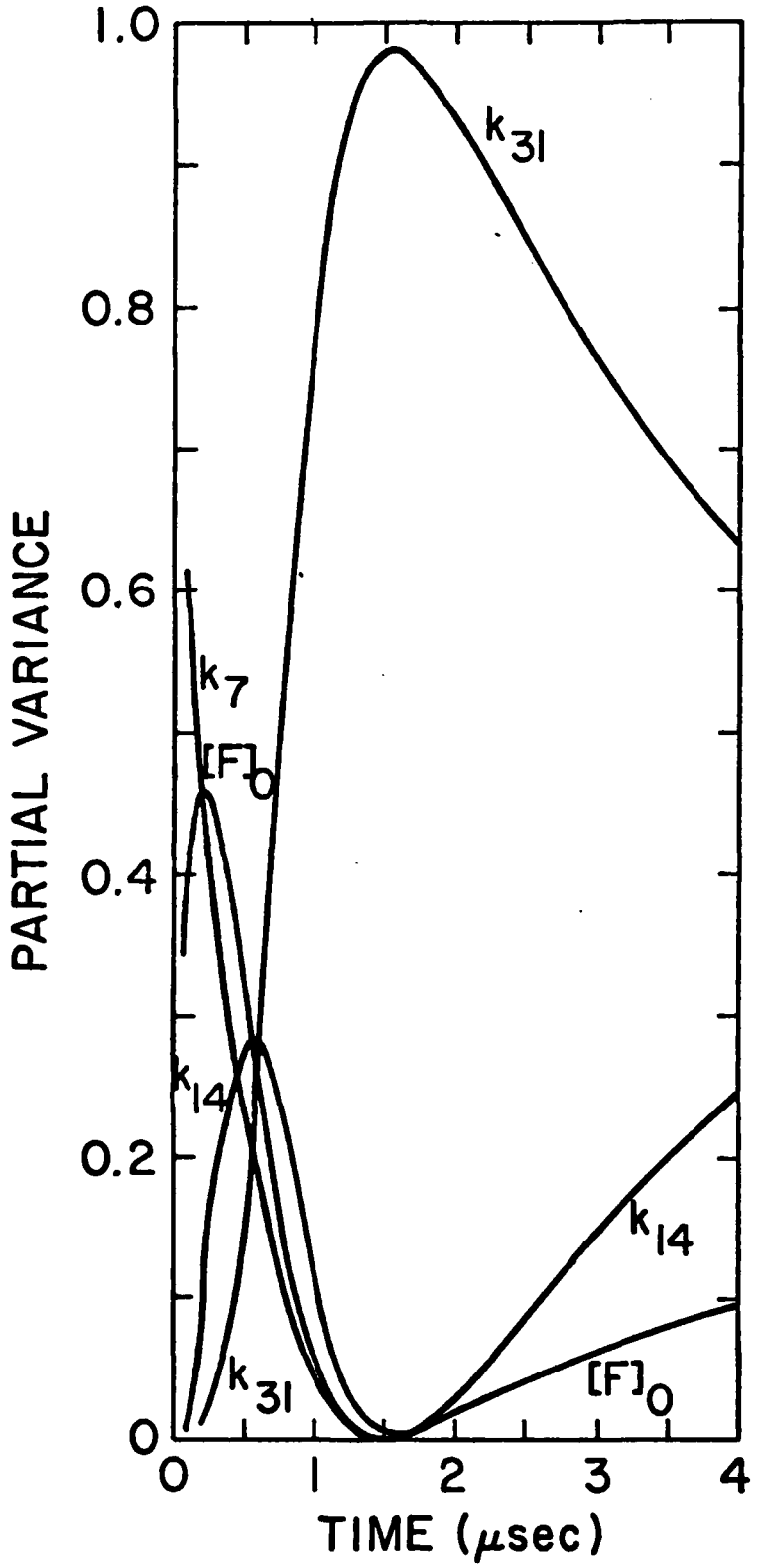

1.0
0.8
0.6
0.4
0.2
0
PARTIAL VARIANCE
0
1
2
3
4
TIME (μsec)
k31
k7
[F]0
k14
k31
k14
[F]0

Fig. 7

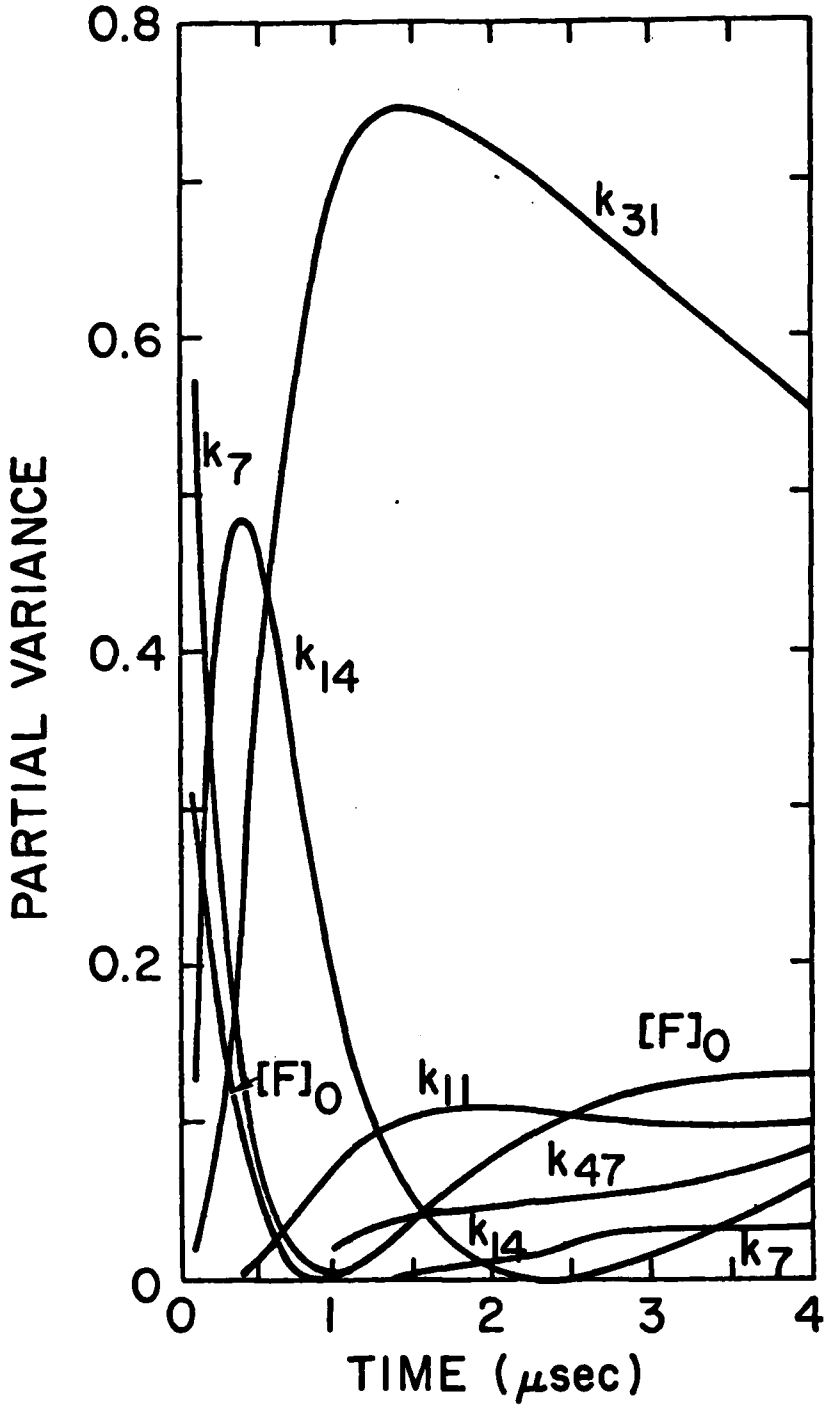
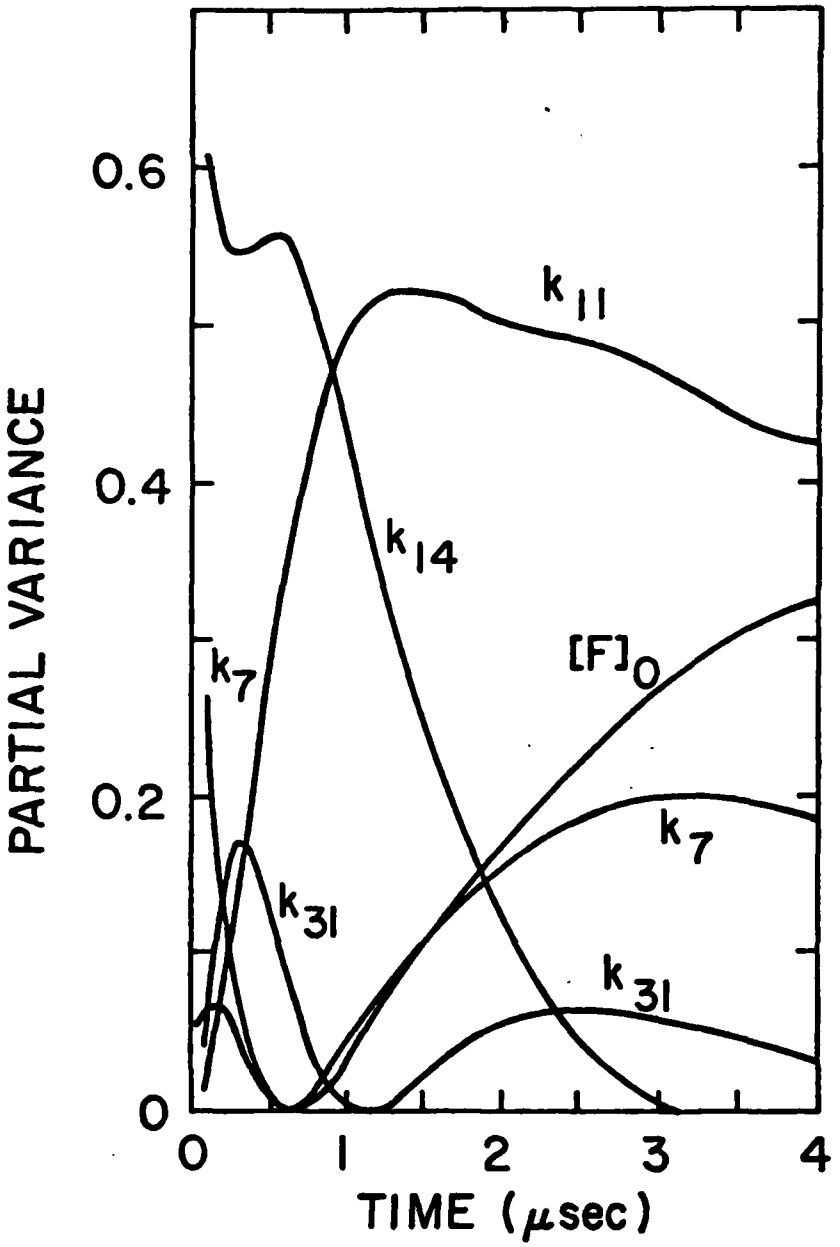
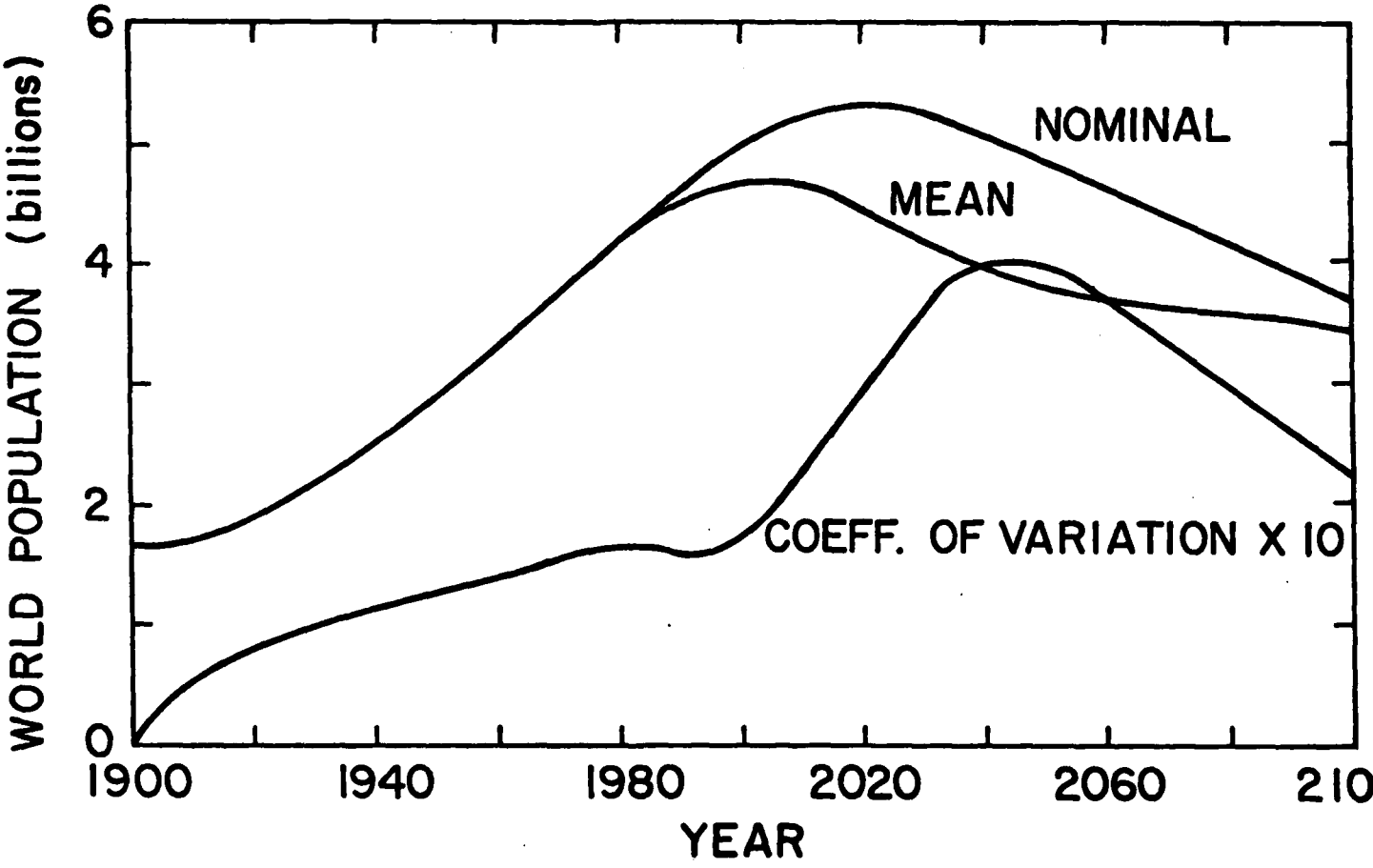
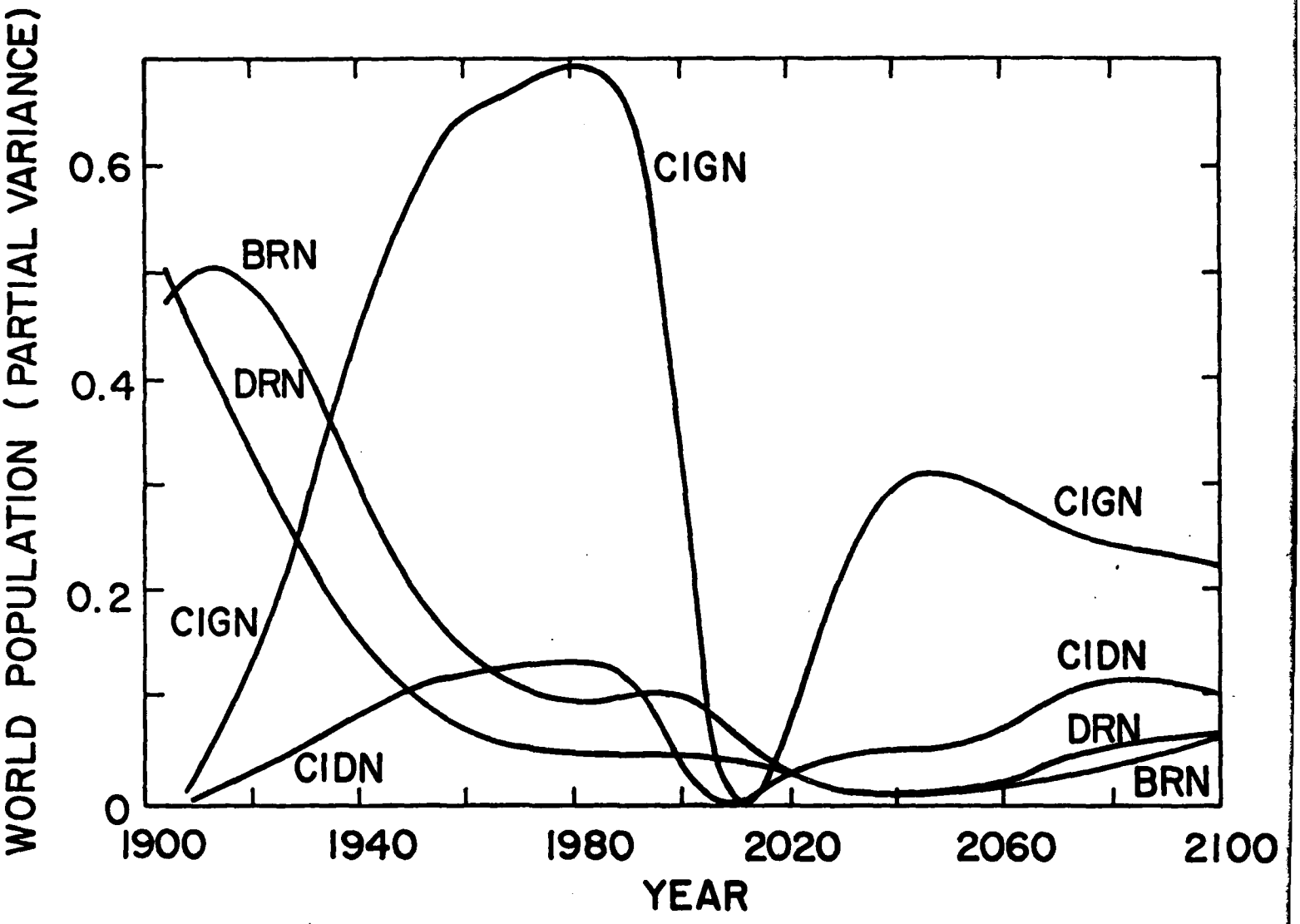
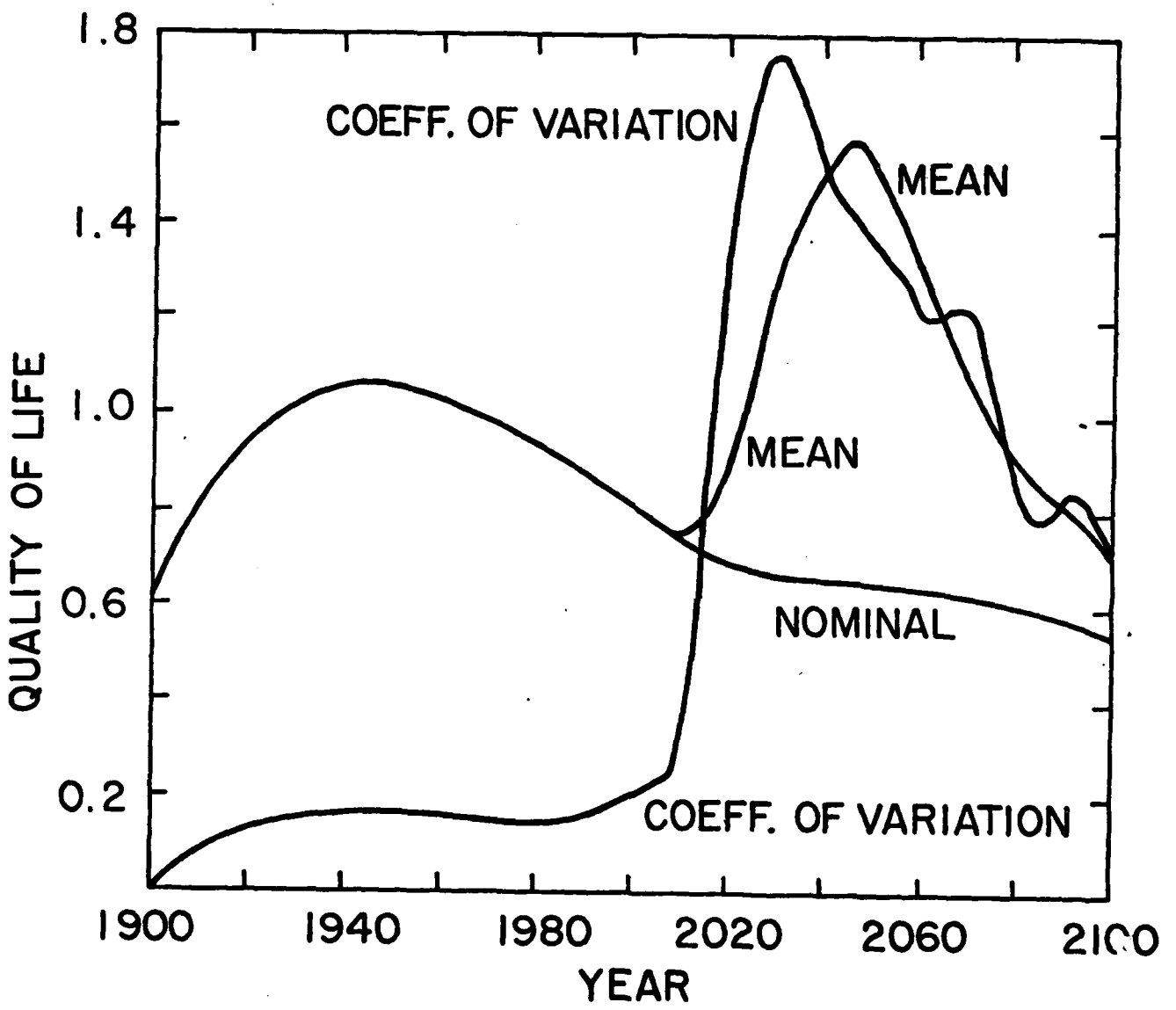

0.8
0.6
0.4
0.2
0
PARTIAL VARIANCE
0
1
2
3
4
TIME (μsec)
k31
k7
k14
[F]0
k11
[F]0
k47
k14
k7

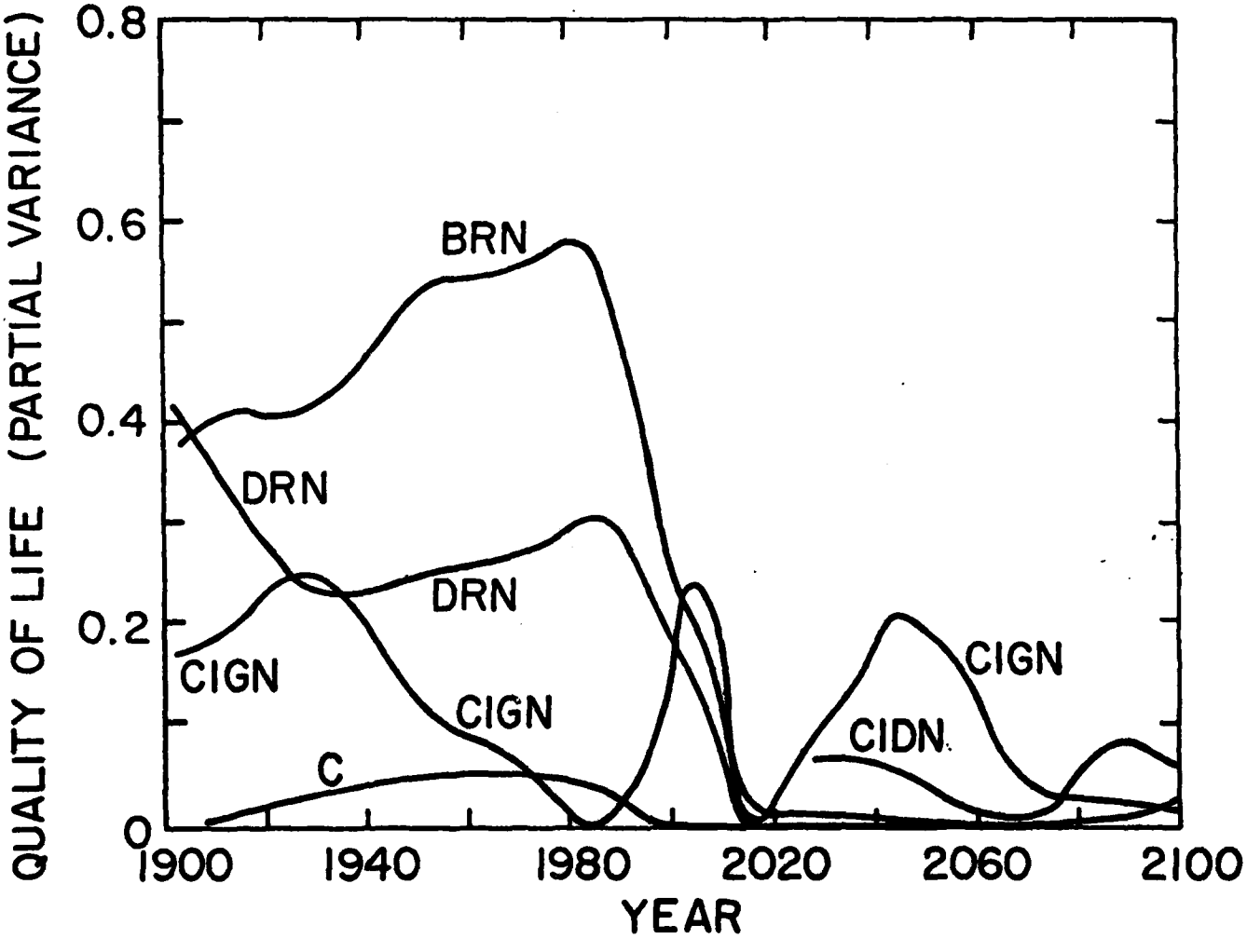
Fig. 8

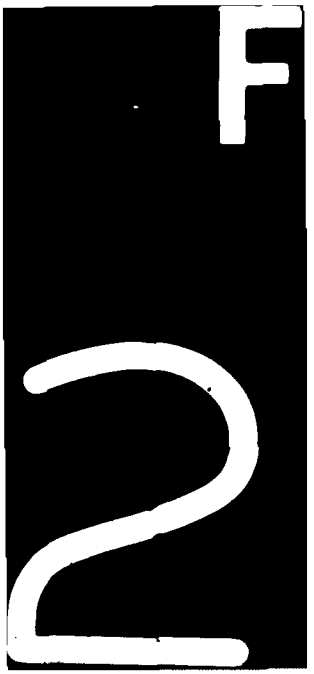

0.6
0.4
0.2
0
PARTIAL VARIANCE
0
1
2
3
4
TIME (μsec)
k11
k14
k7
[F]0
k7
k31
k31


WORLD POPULATION (billions)
6
4
2
0
NOMINAL
MEAN
COEFF. OF VARIATION X 10
1900
1940
1980
2020
2060
210
YEAR


WORLD POPULATION (PARTIAL VARIANCE)
0.6
0.4
0.2
0
BRN
DRN
CIGN
CIGN
CIDN
CIGN
CIDN
DRN
BRN
1900
1940
1980
2020
2060
2100
YEAR


1.8
1.4
1.0
0.6
0.2
QUALITY OF LIFE
COEFF. OF VARIATION
MEAN
MEAN
NOMINAL
COEFF. OF VARIATION
1900
1940
1980
2020
2060
2100
YEAR


QUALITY OF LIFE (PARTIAL VARIANCE)
0.8
0.6
0.4
0.2
0
BRN
DRN
DRN
CIGN
CIGN
C
CIGN
CIDN
1900
1940
1980
2020
2060
2100
YEAR


F
2