

175 Q11  
submitted to: Computers and Chemical Engineering, 1980

*Unpub*

GLOBAL SENSITIVITY ANALYSIS -  
A COMPUTATIONAL IMPLEMENTATION OF THE  
FOURIER AMPLITUDE SENSITIVITY TEST (FAST)

Gregory J. McRae  
James W. Tilden  
John H. Seinfeld\*

Environmental Quality Laboratory  
California Institute of Technology  
Pasadena, California 91125

ABSTRACT

This paper describes a computational implementation of the Fourier Amplitude Sensitivity Test (FAST) and illustrates its use with a sample problem. The FAST procedure is ideally suited to the task of determining the global sensitivity of nonlinear mathematical models subjected to variations of arbitrary size in either the system parameters or initial conditions. A FORTRAN computer program, capable of performing sensitivity analyses of either algebraic or differential equation systems is described.

\*Department of Chemical Engineering

## SCOPE

In virtually all branches of science and engineering, descriptions of phenomena lead to differential equations of substantial complexity. The complexity of such models makes it difficult to determine the effect uncertainties in physical parameters have on their solutions. Traditionally, the analysis of the sensitivity of models to small perturbations in parameters is called *local sensitivity analysis*. When a measure of the sensitivity of the solution to variations of a parameter is combined in an appropriate manner with a measure of the actual degree of uncertainty in the parameter's value, it may then be determined which parameters, through both their sensitivity and uncertainty, have the most influence on the solution. Such a procedure can be called a *global sensitivity analysis*.

Conventional global sensitivity analysis techniques have generally been based on either a pattern search or Monte Carlo technique. Pattern search and Monte Carlo approaches can become extremely time consuming and expensive as the number of parameters becomes large.

The Fourier Amplitude Sensitivity Test (FAST) technique associates each uncertain parameter with a specific frequency in the Fourier transform space of the system. The system sensitivities are then determined by solving the system equations for discrete values of the Fourier transform variable and then computing the Fourier coefficients associated with each parameter frequency. This approach allows nonlinear global sensitivities of systems subjected to large parameter variations to be determined in a practical and efficient manner.

## CONCLUSIONS AND SIGNIFICANCE

Because of the complex nature of many physical and chemical systems, an integral element of any modeling study should be a formal assessment of the effects of uncertainties in the parameterization of the physical processes. In this paper particular attention is given to the Fourier Amplitude Sensitivity Test (FAST) for examining the global sensitivity of nonlinear mathematical models. The FAST technique allows arbitrarily large variations in either system parameters or initial conditions.

The computer program presented here provides a general framework for implementation of the FAST method. When combined with a user supplied subroutine for the specific system of interest, the FAST program computes the sensitivities of the system outputs to the parameter variations specified by the user. The method is illustrated by on an example involving a simple autocatalytic reaction mechanism. x

## 1. INTRODUCTION

A variety of chemical engineering phenomena are described by lengthy and complex mathematical models. It is often desirable to determine the effect of uncertainties in system parameters on the system behavior and to determine which parameters are most influential. The complexity of many models makes it difficult to determine the effect uncertainties in physical and chemical parameters have on solutions. When a measure of the sensitivity of the solution to variations of a parameter is combined in an appropriate manner with a measure of the degree of uncertainty in the parameter's value, one may then determine which parameters, through both their sensitivity and uncertainty, have the most influence on predicted system behavior. Such a study can be termed a *sensitivity/uncertainty analysis* or a *global sensitivity analysis*.

Consider a system that is described by a set of  $n$  coupled ordinary differential equations containing  $m$  parameters,  $k_1, k_2, \dots, k_m$ ,

$$\frac{dx}{dt} = f(x; k) \quad (1)$$

where  $x$  is the  $n$ -dimensional vector of the system state and  $k$  is the  $m$ -dimensional parameter vector. A basic measure of the effect of uncertainties in  $k$  on  $x(t)$  is the deviation in  $x$  caused by a variation in  $k$ ,  $\Delta x(t; k) = x(t; \bar{k} + \Delta k) - x(t; \bar{k})$ , where  $x(t; \bar{k})$  denotes the solution of (1) at time  $t$  with  $k = \bar{k}$ . Taylor's theorem can be invoked to express the deviation in state variable  $i$  as

$$x_i(t; \bar{k} + \Delta k) = x_i(t; \bar{k}) + \sum_{j=1}^m \frac{\partial x_i}{\partial k_j} \Delta k_j + O((\max \Delta k_j)^2) \quad (2)$$

The partial derivatives  $\partial x_i(t)/\partial k_j$ ,  $i = 1, 2, \dots, n$ ,  $j = 1, 2, \dots, m$  are the so-called *sensitivity coefficients*. Much of the work on sensitivity analysis has

been concerned with calculation of these sensitivity coefficients. Sensitivity analysis techniques that rely on calculation of the sensitivity coefficients are strictly applicable only to small parameter variations since the higher order terms in (2) are neglected.

Although the sensitivity coefficients  $\partial x_i / \partial k_j$  provide direct information on the effect of a small variation in each parameter about its nominal value  $\bar{k}_j$  on each state variable, they do not indicate the effect of simultaneous, large variations in all parameters on the state variables. An analysis that accounts for simultaneous parameter variations of arbitrary magnitude can be termed a global sensitivity analysis. The sensitivity coefficients are local gradients in the multidimensional parameter space at the nominal value  $\underline{k}$ . A technique that considers the effect of simultaneous parameter variations over their actual expected ranges of uncertainty produces an average measure of sensitivity over the entire admissible region of variation and thus provides an essentially different measure of sensitivity than that of the sensitivity coefficients. Therefore, both types of analysis are useful in studying the behavior of a system.

Figure 1 shows schematically a hypothetical solution surface  $x_i(t; \underline{k})$  over the domain of uncertainty of two parameters,  $k_1$  and  $k_2$ . The nominal parameter values are  $\bar{k}_1$  and  $\bar{k}_2$ , and the assumed upper and lower limits of variation are indicated producing the domain of uncertainty in the  $k_1$ - $k_2$  plane. The resulting range of uncertainty in  $x_i$  is also indicated. The surface shown in Figure 1 is that at a certain time  $t$ . Generally the variations in the solutions  $x_i(t)$ ,  $i = 1, 2, \dots, n$  must be considered as a function of time. The point Q on the solution surface represents the magnitude of the solution  $x_i$  at time  $t$  with both parameters at their nominal, or best guess, values. Varying both

parameters over the full domain of uncertainty generates the two-dimensional solution surface that changes as  $t$  changes. The sensitivity coefficients,  $\partial x_i / \partial k_1$  and  $\partial x_i / \partial k_2$ , evaluated at  $\bar{k}_1$  and  $\bar{k}_2$  represent the slopes of the surface in the two coordinate directions at point  $Q$ . A local sensitivity analysis would focus on calculation of these two derivatives and their time variation. For small displacements about the nominal values, the tangent plane at  $Q$  differs from the actual solution surface only by a small amount. In this regime the sensitivity coefficients indicate to which parameter the solution is most sensitive. The sensitivity coefficients at point  $Q$  do not contain information on the behavior of the surface away from  $Q$  nor do they indicate the full range of variation of  $x_i$  in the domain of uncertainty of the parameters. The global sensitivity analysis is concerned with assessing the behavior of the entire solution surface of  $x_i$  over the domain of uncertainty of the two parameters.

If we have some knowledge of the probability distributions of the two parameters,  $p(k_1)$  and  $p(k_2)$ , the probability distribution for  $x_i$  can in principle be computed. From the probability distribution of  $x_i$ , certain statistical properties such as the expected value,

$$\langle x_i(t) \rangle = \int_{k_2^{\min}}^{k_2^{\max}} \int_{k_1^{\min}}^{k_1^{\max}} x_i(t; k_1, k_2) p(k_1) p(k_2) dk_1 dk_2 \quad (3)$$

and the variance,

$$\sigma_i^2(t) = \langle x_i(t)^2 \rangle - \langle x_i(t) \rangle^2 \quad (4)$$

where

$$\langle x_i^2(t) \rangle = \int_{k_2^{\min}}^{k_2^{\max}} \int_{k_1^{\min}}^{k_1^{\max}} x_i(t; k_1, k_2)^2 p(k_1) p(k_2) dk_1 dk_2 \quad (5)$$

can be computed.

In Figure 2 given assumed probability distributions for each parameter, a hypothetical probability distribution for the solution is shown. Note that the best value of each parameter, the nominal value, may differ in general from either the most likely value or the mean value. Likewise, the mean value of the solution,  $\langle x_i(t) \rangle$  may not correspond to the value at the nominal parameter values, i.e. point Q.

Whether or not the probability distributions for  $k_1$  and  $k_2$  are given, the solution surface for  $x_i$  can be determined by systematically selecting points in the domain of uncertainty of  $k_1$  and  $k_2$  and solving the system to determine  $x_i(t; k_1, k_2)$ . This approach is indicated in Figure 3. A sensitivity/uncertainty analysis necessitates some form of sampling over the domain of uncertainty of the parameters.

Figure 3 is a schematic illustration of the Monte Carlo method of sensitivity analysis. A random number generator is used to select values of the uncertain parameters within the domain of uncertainty. The system is then solved for each of the parameter combinations randomly selected. The values of  $x_i(t; k)$  thus computed are analyzed by standard statistical methods. The distribution of values obtained is shown in Figure 3 as a histogram with mean value  $\langle x_i \rangle$ . The randomly selected points in the domain of uncertainty of the parameters can be chosen according to any prescribed probability density functions for the parameters. No special programming is required, only that needed to select the parameter values and analyze the solutions statistically.

This paper is devoted to a pattern search procedure for global sensitivity analysis that is an alternative to the Monte Carlo method illustrated in Figure 3. The method is called the Fourier Amplitude Sensitivity Test (FAST) and was originally developed by Shuler, Cukier and coworkers [1-4].

In the next section the mathematical basis of the FAST method is outlined. Then in Section 3 its computational implementation is described. Section 4 contains the description of the computer program and its operation. An example drawn from chemical kinetics is given in Section 5 to illustrate the use of the program.



## 2. MATHEMATICAL BASIS OF THE FAST METHOD

The basic problem is to determine the sensitivity of each  $x_i$  to simultaneous variations in all the parameters  $\{k_j\}$ . This is done by considering that the  $\{k_j\}$  have a distribution of values resulting from either imprecision or uncertainty in their definition. Under these conditions, the ensemble mean for  $x_i$  is given by the generalization of (3),

$$\langle x_i \rangle = \int \cdots \int x_i(k_1, k_2, \dots, k_m) P(k_1, k_2, \dots, k_m) dk_1 dk_2, \dots dk_m \quad (6)$$

where  $P$  is the  $m$ -dimensional probability density for  $k$ .

The central idea of the FAST method is to convert the  $m$ -dimensional integral (6) into a one dimensional form by using the transformation,

$$k_\ell = G_\ell[\sin(\omega_\ell s)] ; \quad \ell = 1, 2, \dots, m \quad (7)$$

For an appropriate set of functions  $\{G_\ell\}$ , it can be shown that [ 5 ]

$$\bar{x}_i = \lim_{T \rightarrow \infty} \frac{1}{2T} \int_{-T}^T x_i[k_1(s), k_2(s), \dots, k_m(s)] ds \quad (8)$$

This relationship will hold only if the frequency set,  $\{\omega_\ell\}$ , is incommensurate, i.e.

$$\sum_{i=1}^m \gamma_i \omega_i = 0 \quad (9)$$

For an integer set of  $\{\gamma_i\}$  if and only if  $\gamma_i = 0$  for every  $i$ . The functions  $\{G_\ell\}$  need to be chosen so that the arc length,  $ds$ , is proportional to  $P(k_1, k_2, \dots, k_m) dk_\ell$  for all  $\ell$ . The transformation then results in a search curve that samples the parameter space in a manner consistent with the statistics described by  $P(K_1, k_2, \dots, k_m)$ .

The parametric curve defined by (7) is termed a search curve, and  $s$  is termed the search variable. As  $s$  is varied, (7) traces out a space filling curve in the parameter space. If it were possible to use an incommensurate frequency set, the curve would never close upon itself and would pass arbitrarily close to every point in the parameter space. This result is a consequence of Weyl's theorem. When integer frequencies are used, it is not possible to obtain a truly incommensurate frequency set and the search curves take on the appearance of multi-dimensional Lissajous curves. The use of higher frequencies results in successively longer search curves. Two examples are shown in Figures 4 and 5.

The length of the search curve and the density of sample points is considerably greater in the second case.

Practical considerations dictate that an integer rather than an incommensurate frequency set must be used. This introduces two types of error. First, the search curve is no longer space-filling, i.e., it does not pass arbitrarily close to any point in the  $k$ -space; secondly, the fundamental frequencies used to describe the set  $\{k_\ell\}$  will have harmonics that interfere with one another. However, the difference between  $\bar{x}$  and  $\langle x \rangle$  for a well chosen integer frequency set can be made arbitrarily small [ 2,3].

An integer frequency set results in a periodic search curve that becomes a closed path in the  $s$ -space. When  $s$  is varied between  $-\pi$  and  $+\pi$ , the entire search curve is traversed. The periodicity of the  $\{k_\ell\}$  then implies that the Fourier coefficients

$$A_{p\omega_\ell}^{(i)} = \frac{1}{2\pi} \int_{-\pi}^{\pi} x_i[k_1(s), \dots, k_m(s)] \cos(p\omega_\ell s) ds \quad (10)$$

$$p = 0, 1, 2, \dots$$

$$B_{p\omega_\ell}^{(i)} = \frac{1}{2\pi} \int_{-\pi}^{\pi} x_i[k_1(s), \dots, k_m(s)] \sin(p\omega_\ell s) ds \quad (11)$$

$$p = 1, 2, \dots$$

are a measure of the sensitivity of the  $x_i$  output function to the  $k$ th uncertain parameter. For instance, in the case where  $x_i$  is totally insensitive to a given parameter, the coefficients corresponding to that parameter would be zero.

The ensemble average,

$$\langle x_i \rangle = \frac{1}{2\pi} \int_{-\pi}^{\pi} x_i[k_1(s), \dots, k_m(s)] ds \quad (12)$$

can be expressed in terms of the Fourier coefficients as

$$\langle x_i \rangle^2 = A_0^{(i)^2} + B_0^{(i)^2} = A_0^{(i)^2} \quad (13)$$

The variance of  $x_i$  is then

$$\sigma_i^2 = \frac{1}{2\pi} \int_{-\pi}^{\pi} x_i^2 ds - \langle x_i \rangle^2 \quad (14)$$

Parseval's theorem can then be used to determine the variance of  $x_i$ , i.e.

$$\langle x_i^2 \rangle = \frac{1}{2\pi} \int_{-\pi}^{\pi} x_i^2(s) ds = \sum_{j=-\infty}^{\infty} \left\{ A_j^{(i)^2} + B_j^{(i)^2} \right\} \quad (15)$$

The variance and harmonics due to  $\omega_\ell$  are expressed by

$$\sigma_{\omega_\ell}^{(i)^2} = 2 \sum_{p=1}^{\infty} \left[ A_{p\omega_\ell}^{(i)^2} + B_{p\omega_\ell}^{(i)^2} \right] \quad (16)$$

The normalized sensitivity measure, the partial variance,  $S_{\omega_\ell}^{(i)}$ , is then defined by the ratio of the variance due to frequency  $\omega_\ell$  to the total variance,

$$S_{\omega_\ell}^{(i)} = \frac{\left( \sigma_{\omega_\ell}^{(i)} \right)^2}{\left( \sigma^{(i)} \right)^2} \quad (17)$$

Thus the  $\{S_{\omega_\ell}^{(i)}\}$  represent an ordered measure of the sensitivity of the system to each of the  $\{k_\ell\}$  parameters.

The FAST method requires that the system be solved to produce the output state variable values, the Fourier coefficients and subsequently the partial variances.

### 3. COMPUTATIONAL IMPLEMENTATION OF THE FAST ALGORITHM

Application of the FAST method requires the numerical evaluation of the Fourier coefficients,  $A_{p\omega_\ell}^{(i)}$  and  $B_{p\omega_\ell}^{(i)}$ . This in turn requires the  $x_i$  be evaluated as  $s$  ranges over  $[-\pi, \pi]$ . Restricting the frequency set to odd integers reduces the range of  $s$  to  $[-\frac{\pi}{2}, \frac{\pi}{2}]$ . In this case

$$\begin{aligned} x(\pi-s) &= x(s) \\ x(-\pi+s) &= x(-s) \\ x\left(\frac{\pi}{2} + s\right) &= x\left(\frac{\pi}{2} - s\right) \\ x\left(-\frac{\pi}{2} + s\right) &= x\left(-\frac{\pi}{2} - s\right) \end{aligned} \quad (18)$$

and the Fourier coefficients can be expressed as:

$$A_j^{(i)} = \begin{cases} 0 & ; \quad j \text{ odd} \\ \frac{1}{\pi} \int_0^{\pi/2} [x_i(s) + x_i(-s)] \cos jsds & ; \quad j \text{ even} \end{cases} \quad (19)$$

and

$$B_j^{(i)} = \begin{cases} 0 & ; \quad j \text{ even} \\ \frac{1}{\pi} \int_0^{\pi/2} [x_i(s) - x_i(-s)] \sin jsds & ; \quad j \text{ odd} \end{cases} \quad (20)$$

The actual number of points at which the system must be evaluated can be derived from the Nyquist criterion [ 6 ], and is found to be

$$r \geq N\omega_{\max} + 1 \quad (21)$$

Where  $r$  is the number of solution points and  $N$  an even integer.

For convenience in calculating the Fourier coefficients, the additional condition

$$2r = 4q + 2 \quad (22)$$

where  $q$  is an integer is also imposed. The values of  $s$  are taken to be equally spaced throughout the range  $[-\frac{\pi}{2}, \frac{\pi}{2}]$ , and the discrete points at which  $x_i$  is calculated in the Fourier space are given by

$$s_j = \frac{\pi}{2} \left[ \frac{2j-r-1}{r} \right] \quad j = 1, 2, \dots, r \quad (23)$$

The following difference expressions for Fourier coefficients can be derived by a simple numerical quadrature technique [4,7],

$$A_j^i = 0 \quad (j \text{ odd}) \quad (24)$$

$$B_j^i = 0 \quad (j \text{ even}) \quad (25)$$

$$A_j^i = \frac{1}{2q+1} \left[ x_0^i + \sum_{k=1}^q (x_k^i + x_{-k}^i) \cos \left( \frac{\pi j k}{2q+1} \right) \right]; \quad (j \text{ even}) \quad (26)$$

$$B_j^i = \frac{1}{2q+1} \left[ \sum_{k=1}^q (x_k^i - x_{-k}^i) \sin \left( \frac{\pi j k}{2q+1} \right) \right]; \quad (j \text{ odd}) \quad (27)$$

where  $x^i$  replaces  $x_i$  for notational purposes.

Interference between the frequencies will occur as a result of this numerical evaluation when

$$q\omega_j = p\omega_\ell \quad [\text{Mod}(N\omega_{\max} + 1)] \quad (28)$$

which results in

$$|A_{p\omega_\ell}^{(i)}|^2 + |B_{p\omega_\ell}^{(i)}|^2 = |A_{q\omega_j}^{(i)}|^2 + |B_{q\omega_j}^{(i)}|^2 \quad (29)$$

since

$$\sin \left[ \frac{\pi q \omega_j}{N \omega_{\max} + 1} \right] = \pm \sin \left[ \frac{\pi p \omega_\ell}{N \omega_{\max} + 1} \right] \quad (30)$$

and

$$\cos \left[ \frac{\pi q \omega_j}{N \omega_{\max} + 1} \right] = \pm \cos \left[ \frac{\pi p \omega_\ell}{N \omega_{\max} + 1} \right] \quad (31)$$

This interference, called aliasing, is eliminated when

$$r \omega_\ell \leq N \omega_{\max} + 1. \quad (32) \quad \times$$

N is therefore the maximum number of Fourier coefficients that may be retained in calculating the partial variances without interferences between the assigned frequencies. The expression for  $S_{\omega_\ell}^{(i)}$  then becomes

$$S_{\omega_\ell}^{(i)} = \frac{2}{\sigma_i^2} \sum_{j=1}^N \left[ |A_{j\omega_\ell}^{(i)}|^2 + |B_{j\omega_\ell}^{(i)}|^2 \right] \quad (33)$$

Interference will also result from the use of an integer frequency set if the number of Fourier coefficients N used in the summation (33) is greater than or equal to the smallest frequency. To illustrate this consider (33) for the frequencies  $\omega_\ell$  and  $\omega_{\ell'}$ ,

$$\begin{aligned} S_{\omega_\ell}^{(i)} &= A_{\omega_\ell}^{(i)2} + B_{\omega_\ell}^{(i)2} + \dots + A_{N\omega_\ell}^{(i)2} + B_{N\omega_\ell}^{(i)2} \\ S_{\omega_{\ell'}}^{(i)} &= A_{\omega_{\ell'}}^{(i)2} + B_{\omega_{\ell'}}^{(i)2} + \dots + A_{N\omega_{\ell'}}^{(i)2} + B_{N\omega_{\ell'}}^{(i)2} \end{aligned}$$

If  $N \geq \omega_1$ , terms in the series for  $S_{\omega_\ell}^{(i)}$  and  $S_{\omega_{\ell'}}^{(i)}$  become identical. For example, if  $N = \omega_1$ , and if  $\omega_{\ell'} > \omega_\ell$ , there will be a term in the  $S_{\omega_{\ell'}}^{(i)}$  series for which

$$A_{\omega_1 \omega_\ell}^{(i)} = A_{j \omega_\ell}^{(i)}$$

In such a case, the effect of the variation of parameter  $\ell$  enters spuriously into the partial variance for the variation of parameter  $\ell'$ .

In general, the interference between the higher harmonics will be eliminated when

$$N < \omega_{\min} - 1. \quad (37)$$

$N$  is also related to the number of function evaluations required by (21), so it is desirable to use the minimum possible value, which is  $N=2$ . Then a minimum frequency of at least three is sufficient to remove any harmonic interference effects from the partial variances. The final expression for the partial variances then becomes

$$S_{\omega_\ell}^{(i)} = \frac{2}{\sigma_i^2} \left\{ \left| B_{1\omega_\ell}^{(i)} \right|^2 + \left| A_{2\omega_\ell}^{(i)} \right|^2 \right\} \quad (38)$$

The choice of  $N=2$  restricts the number of terms in the series to two. This is generally sufficient because the magnitude of the higher order terms in the Fourier series tend to decrease rapidly.

Implementation of the FAST technique also requires the selection of a frequency set, which can be done recursively using

$$\omega_1 = \Omega_n \quad (39)$$

$$\omega_i = \omega_{i-1} + d_{n+1-i} \quad (40)$$

as described in Cukier et al. [ 4 ]. The  $\Omega_n$  and  $d_n$  we have used are tabulated in Table 1.

The final step in the FAST implementation is the determination of the transformation functions  $\{G_\ell\}$  that determine the actual search curve traversed in  $s$ -space. If the probabilities of occurrence for the parameters  $\{k_\ell\}$  are



independent, the probability density describing their effects has the form,

$$P(k_1, k_2, \dots, k_m) = P_1(k_1)P_2(k_2) \dots P_m(k_m) \quad (41)$$

In this case it can be shown that the transformation functions must obey the relation [ 5 ]

$$\pi(1 - x^2)^{1/2} P_\ell(G_\ell) \frac{dG_\ell(x)}{dx} = 1 \quad (42)$$

with the initial conditions  $G_\ell(0) = 0$ . A tabulation of three different search curve formulations and their transformation functions is given in Table 2.

The parameter probability distributions used to derive these curves are described in Cukier et al.[3]. The first search curve is suitable for cases with small variations in the uncertain parameters while the second and third are applicable to cases with large variations.

#### 4. PROGRAM DESCRIPTION AND OPERATION

A flowchart of the FAST program is shown in Figure 6. There are two user interfaces with the program. One is the input data set which contains the following information; program description cards, control cards, analysis times (optional), and parameter cards. The second interface is a user supplied subroutine, called F, that calculates the state variable values for a given parameter combination. When the state variables must be calculated numerically, the user must also provide a subroutine to perform this function. For chemical kinetic applications several existing differential equation solvers can be easily adopted.

The input information is stored in an array called P. Subroutines F must access P in the same sequence that the parameters were specified on the input cards. The state variables calculated in the F subroutine are returned in an array named C. The structure of this array is shown in Figure 7. An example of subroutine F for the sample problem in Section 5 is given in Figure 8. The detailed fields and formats for the input file are shown in Table 3.

The default value for the number of analysis times is one, and the default for the number of terms in the partial variance series is two. If this latter default is to be changed, care must be exercised to be sure that the number of points at which  $x$  and the Fourier coefficients are evaluated is also modified so that interferences between the parameters will not occur.

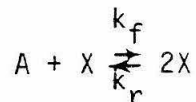
Five files can be accessed during execution of the program. These are described in Table 4. Whenever the option to save the results is used, both file IDOUT and file IDISC must be allocated. IDOUT must be allocated when the reanalysis option is specified, and IDPLT must be allocated when the

option to plot the partial variances is used. ICARD and IPRIN must be allocated at all times.

Several of the arrays used in the FAST program can become quite large for problems involving several parameters, output state variables and/or analysis times. The default sizes for the program arrays are given in Table 5. The program tests the input requests to determine if the default storage is sufficient, if not, the program will terminate and write an error message describing which arrays require enlargement.

## 5. SAMPLE PROBLEM

To illustrate the use of the FAST program, a simple example consisting of a single, autocatalytic reaction,



is considered. The concentration of  $X$  is governed by

$$\frac{d[X]}{dt} = k_f[A][X] - k_r[X]^2$$

$$[X(0)] = [X]_0$$

If we assume that  $[A]$  is constant, the dimensionless concentration

$$[\hat{X}] = \frac{k_r[X]}{k_f[A]}$$

can be defined, and the differential equation solved to yield

$$[\hat{X}] = \left[ 1 - (1 - [\hat{X}]_0^{-1})e^{-k_f[A]t} \right]^{-1}$$

For the purposes of sensitivity analysis, we express  $k_f$  in the Arrhenius form,

$$k_f = B_f e^{-C_f/T}$$

We wish to examine the sensitivity of  $[\hat{X}]$  to  $[\hat{X}]_0$ ,  $[A]$ ,  $B_f$ ,  $C_f$ , and  $T$  from  $t = 0$  to  $t = 2$ . The nominal values and ranges of variation of these five parameters are given in Table 6 .

Figure 9 shows the first-order normalized sensitivity coefficients as a function of time evaluated at the nominal values of Table 4. These are defined by

$$\rho_i(t) = \frac{\left| \frac{\partial \hat{x}}{\partial k_i} \Delta k_i \right|}{\sum_{j=1}^m \left| \frac{\partial \hat{x}}{\partial k_j} \Delta k_j \right|}$$

Figure 10 presents the partial variances for the five parameters as determined by the FAST method with the  $\pm 5$  percent variations of Table 6 using search curve 1 of Table 2. We note first that the first-order sensitivities of  $[\hat{X}]$  to variations in  $[A]$  and  $B_f$  are identical because these two parameters appear as a product in  $[\hat{X}]$ . The same behavior is noted for  $C_f$  and  $T$ . As long as the uncertainty ranges chosen for these two sets of parameters are the same, the partial variances of  $[A]$  and  $B_f$  and  $C_f$  and  $T$  are identical, as seen in Figure 10. The qualitative results of both the first-order sensitivity coefficients and the FAST partial variances are the same, although the relative magnitudes differ somewhat. A difference in relative magnitudes is expected since the first-order sensitivity coefficients are computed at the nominal values, whereas the FAST partial variances involve simultaneous variation of all five parameters over their range of uncertainty, in this case  $\pm 5$  percent. Both sets of calculations show that  $[\hat{X}]$  is most sensitive to  $[\hat{X}]_0$  for  $0 \leq t \leq 1.1$ . For  $t > 1.1$ ,  $[\hat{X}]$  is most sensitive to  $[A]$  and  $B_f$ . Note that the FAST method shows that the sensitivity of  $[\hat{X}]$  to  $[\hat{X}]_0$  close to  $t = 0$  is larger than indicated by the first-order sensitivity coefficient.

ACKNOWLEDGMENT

- This work was supported by U.S. Environmental Protection Agency grant R805537.

# NOMENCLATURE

$A$	constant chemical species
$A_j^{(i)}$	jth Fourier cosine coefficient for the ith state variable
$B_F$	pre-Arrhenius rate term
$B_j^{(i)}$	jth Fourier sine coefficient for the ith state variable
$C_F$	activation energy germ
$d_n$	frequency set generation parameter
$f(x;k)$	general system function
$G_\ell$	transformation function
$k_f$	forward rate constant
$k_i$	ith uncertain parameter
$k_i^\ell$	lower limit of ith uncertain parameter
$k_i^u$	upper limit of ith uncertain parameter
$k_r$	reverse rate constant
$m$	number of uncertain parameters
$n$	number of state variables
$N$	number of Fourier
$P(k)$	probability distribution of the uncertain parameters $\underline{k}$
$q$	quadrature index
$r$	number of numerical solution points
$r^\ell$	ratio of parameter lower limit and mean value
$r^u$	ratio of parameter upper limit and mean value
$s$	Fourier space variable
$s_j$	discrete Fourier space variable

$s_j^{(i)}$	partial sensitivity of the $i$ th state variable to the $j$ th uncertain parameter
$T$	temperature
$x$	state variable
$x_k^i$	the value of the $i$ th state variable at the $k$ th numerical solution point
$X$	chemical species
$\hat{X}$	normalized chemical species
$\alpha_j$	search curve parameter
$\beta_j$	search curve parameter
$\sigma_i^2$	partial variance of the $i$ th state variable
$\rho_i$	normalized linear sensitivity coefficient for the $i$ th state variable
$\omega_j$	Fourier frequency assigned to the $j$ th parameter
$\bar{v}_j$	nominal value of the $j$ th uncertain parameter
$\Omega_n$	frequency set generation parameter
$\langle \rangle$	ensemble average quantity
$-$	time average quantity



# REFERENCES

1. R. I. Cukier, C. M. Fortuin, K. E. Shuler, A. G. Petschek and J. H. Schaibly, J. Chem. Phys. 59 (8), 3873 (1973).
2. J. H. Schaibly and K. E. Shuler, J. Chem. Phys. 59 (8), 3879 (1973).
3. R. I. Cukier, J. H. Schaibly and K. E. Shuler, J. Chem. Phys. 63(3), 1140 (1975).
4. R. I. Cukier, H. B. Levine and K. E. Shuler, J. Comp. Phys. 26(1) 1 (1978).
5. H. Weyl, Amer. J. Math. 60, 889 (1938).
6. K. G. Beauchamp and C. K. Yuen, Digital Methods for Signal Analysis, George Allen and Unwin, London (1979).
7. M. Koda, G. J. McRae and J. H. Seinfeld, Int. J. Chem. Kinetics 11 427 (1979).
8. R. J. Gelinas and J. P. Vajk, Systematic Sensitivity Analysis of Air Quality Simulation Models, Final Report to U.S. Environmental Protection Agency under Contract No. 68-02-2942, Science Applications, Inc., Pleasanton, CA (1978).

Table 1. Parameters Used in Calculating Frequency Sets Free of Interferences to Fourth Order

N	$\Omega_n$	$d_n$	N	$\Omega_n$	$d_n$
1	0	4	26	385	416
2	3	8	27	157	106
3	1	6	28	215	208
4	5	10	29	449	328
5	11	20	30	163	198
6	1	22	31	337	382
7	17	32	32	253	88
8	23	40	33	375	348
9	19	38	34	441	186
10	25	26	35	673	140
11	41	56	36	773	170
12	31	62	37	875	284
13	23	46	38	873	568
14	87	76	39	587	302
15	67	96	40	849	438
16	73	60	41	623	410
17	85	86	42	637	248
18	143	126	43	891	448
19	149	134	44	943	388
20	99	112	45	1171	596
21	119	92	46	1225	216
22	237	128	47	1335	100
23	267	154	48	1725	488
24	283	196	49	1663	166
25	151	34	50	2019	0

Table 2. Search Curves for Fourier Amplitude Sensitivity Test  
Computer Program

APPLICATION	$k_j(s)$	MEAN VALUE $\bar{k}_j$	NOMINAL VALUE $\bar{v}_j$
ADDITIVE VARIATION	$k_j(s) = \bar{k}_j [1 + \bar{v}_j \sin \omega_j s]$	$\frac{k_j^u + k_j^l}{2}$	$\frac{k_j - k_j^l}{k_j + k_j^l}$
EXPONENTIAL VARIATION	$k_j(s) = \bar{k}_j \exp [\bar{v}_j \sin \omega_j s]$	$\sqrt{k_j^u k_j^l}$	$\frac{1}{2} \ln \left( \frac{k_j^u}{k_j^l} \right)$
PROPORTIONAL VARIATION $k_j^u = a \bar{k}_j, k_j^l = \left( \frac{\bar{k}_j}{a} \right)$	$k_j(s) = \bar{k}_j \exp [v_j \sin \omega_j s]$	$\bar{k}_j$	$\ln(a)$
SKEWED VARIATION $k_j > \left( \frac{k_j^u + k_j^l}{2} \right)$	$k_j(s) = v_j \left[ \frac{a_j + \beta_j \sin \omega_j s - 1}{a_j + \beta_j \sin \omega_j s} \right]$	$v_j \left( \frac{a_j - 1}{a_j} \right)$	$a_j = \frac{1}{2} \left[ \frac{r^u}{r^u - 1} + \frac{r^l}{r^l - 1} \right]^b$ $\beta_j = -\frac{a_j (r^u + r^l - 2)}{(r^u - r^l)}$ $v_j = -\bar{k}_j \left[ \frac{r^u + r^l - 2r^u r^l}{r^u + r^l - 2} \right]$

<sup>a</sup>  $k_j^u$  - upper limit for parameter;  $k_j^l$  - lower limit for parameter

<sup>b</sup>  $r^u = k_j^u / \bar{k}_j, r^l = k_j^l / \bar{k}_j$

Table 3. Input Fields and Formats

Problem Description Cards

72A1													
1													72

Col 1-72. Descriptive text. Number of cards is optional. The end of the text is indicated by a \* in col 1 of the last description card.

Control Card

							15I5							
1													75	

Col.	Description
1-5	number of analysis times
6-10	number of input parameters
11-15	number of output state variables
16-20	number of terms in the partial variance sum (default 2)
21-25	option to print amplitudes
26-30	option to print parameter combinations
31-35	option to print state variable outputs
36-40	multiplier N in $N=N_{w_{max}}+1$ (default 2)
41-45	option to print unsorted partial variances
46-50	option to save state variable outputs on disc file
51-55	option to reanalyze state variable outputs
56-60	option to plot partial variances
61-65	option to renormalize partial variances for plotting
66-70	option to print partial variances during reanalysis
71-75	option to print sorted partial variances during plotting

Table 3. Input Fields and Formats (Continued)

Analysis Times (Optional)

F10.0	
1	10

Col	Description
1-10	Analysis time. Number if cards required is determined by the number of analysis times entered in the control card. (These cards may be omitted if the number of analysis times entered on the control card is zero.)

Parameter Card

I5	I5	F10.0	F10.0	50A1
1	6	11		80

Col	Description
1-5	Parameter number. This number is the array index used for the P array in Subroutine F. The frequency assignment is done in the order in which the parameter cards are input. If an alternative frequency assignment is desired, the order in which the parameter cards are input should be changed, but <u>not</u> the parameter number.
6-10	Search curve type 0 = Fixed Parameter 1 = Small Parameter Variation 2 = Large Parameter Variation 3 = Parameter Variation Expressed as Fractional Change
11-20	Lower parameter limit or fixed parameter value
21-30	Upper parameter limit (type 1) or scale factor (types 2 and 3).
31-80	Parameter Description.

Table 4. Files Used by FAST Program

Name	Unit Number	Description
IDOUT	1	Reanalysis file. When the option to save the results is used, the output values are stored on this file. When the reanalysis option is used, the state values from this file are read as input.
IDISC	2	Save file. When the save option is on, all other program information including the partial variances is written to this file for later use.
IDPLT	3	Plot file. All information required for plotting is stored on this file during program execution and read back during the execution of the plot routine.
ICARD	5	User's input file.
IPRIN	6	Output print file.

Table 5. FAST Program Array Default Sizes

Array	Description	Default Size	Size Variable
IVARB	Variable Numbers	100	NVMAX
ITYPE	Variable Types	100	NVMAX
UBAR	Nominal Values	100	NVMAX
PBAR	Mean Values	100	NVMAX
PV	Variances	100	NVMAX
INDEX	Sort Array	100	NVMAX
PARM	Parameter Combinations	100	NVMAX
DESC	Parameter Descriptions	(48,100)	NVMAX
IW	Frequency Set	50	NPMAX
TIME	Analysis Times	50	NTMAX
OUTPT	Parameter Output	200	NOMAX
FI	Output for All Parameter Combinations	2000	NSMAX
NVMAX	Max Number of Input Parameters		100
NPMAX	Max Number of Variable Parameters		50
NTMAX	Max Number of Analysis Times		50
NOMAX	Max Storage for Each Parameter Combination		200
NSMAX	Max Storage for All Parameter Combinations		2000
NEQN	Number of Solutions for Each Combination		no limit
NSTAT	Number of State Variable Outputs		no limit

Table 6. Parameter Variations for Autocatalytic System

Parameter	Nominal Value	Range of Uncertainty (+5%)
$[\hat{X}]_0$	0.15	0.1425 - 0.1575
[A]	1.73	1.644 - 1.817
$B_f$	1.0	0.95 - 1.05
$C_f$	165.0	156.8 - 173.3
T	300.0	285.0 - 315.0



# FIGURE CAPTIONS

- Figure 1. Hypothetical Solution Surface Over the Domain of Uncertainty of Two Parameters (after Gelinas and Vajk, [8].)
- Figure 2. Hypothetical Probability Distribution of Solution Surface Corresponding to the Probability Distributions of the Two Parameters (after Gelinas and Vajk, [8].)
- Figure 3. Monte Carlo Approach to Generating the Solution Surface (after Gelinas and Vajk, [8].)
- Figure 4. Space Filling Search Curve with Frequencies  $\omega_1 = 3$ ,  $\omega_2 = 5$ .
- Figure 5. Space Filling Search Curve with Frequencies  $\omega_1 = 11$ ,  $\omega_2 = 13$ .
- Figure 6. Fourier Amplitude Sensitivity Test Program
- Figure 7. Structure of the Output Array C
- Figure 8. Description of Subroutine F
- Figure 9. First-Order Sensitivity Coefficients for the Reaction  

$$A + X \xrightarrow{k_1} 2X$$
- Figure 10. Partial Variances from the FAST Method for the Reaction  

$$A + X \xrightarrow{k_1} 2X$$

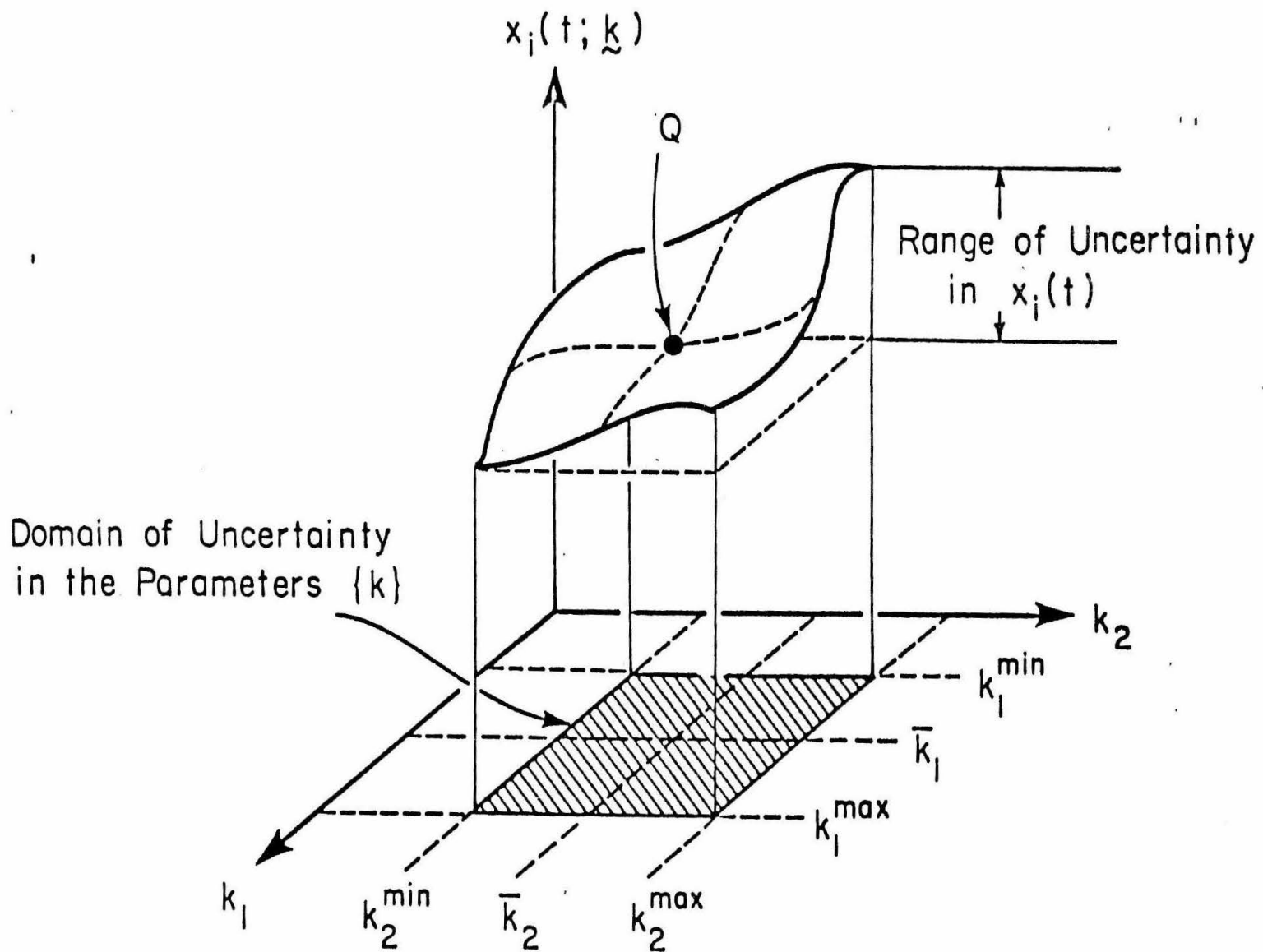


Figure 1. Hypothetical Solution Surface Over the Domain of Uncertainty of Two Parameters (after Gelinas and Vajk, 1978)



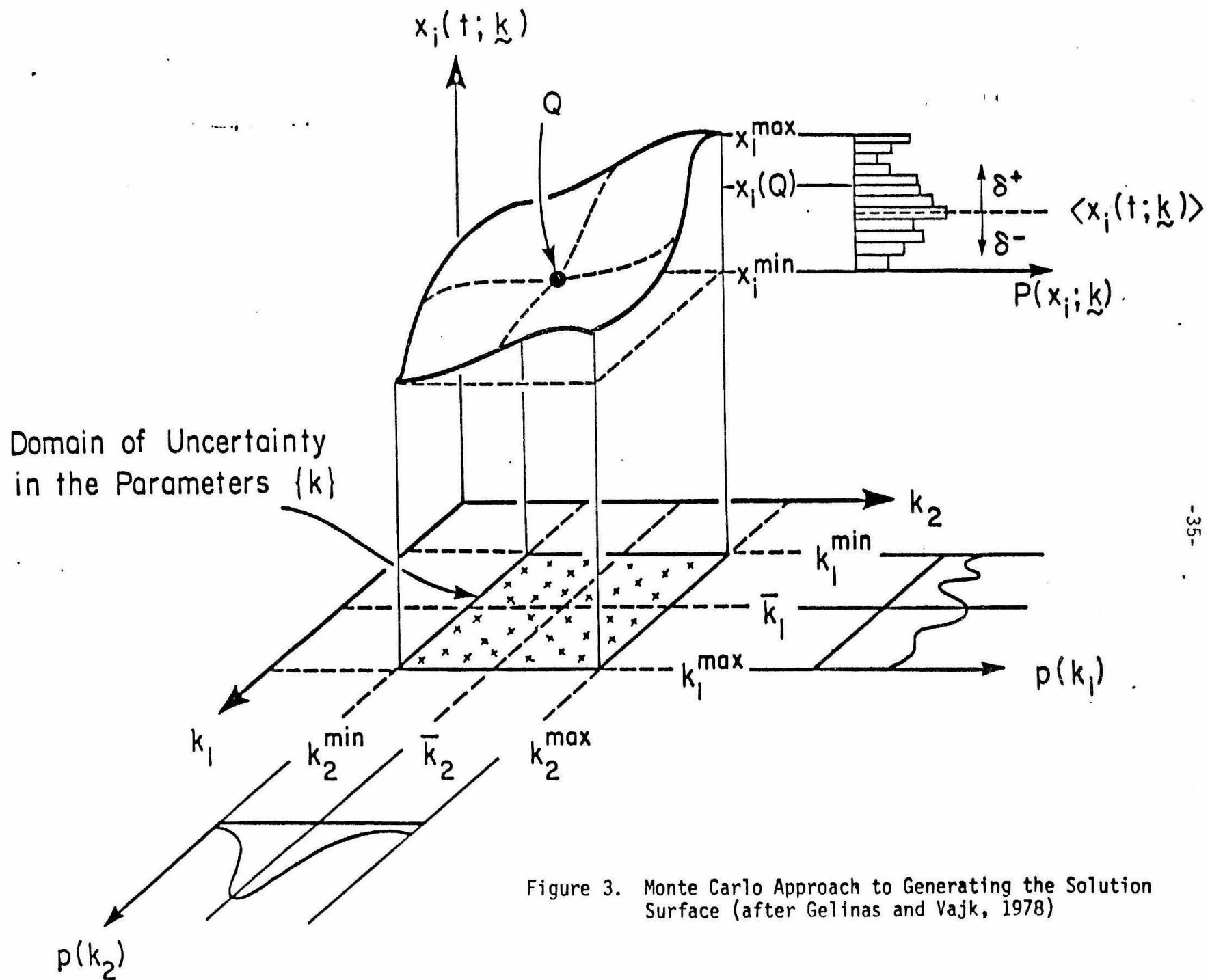
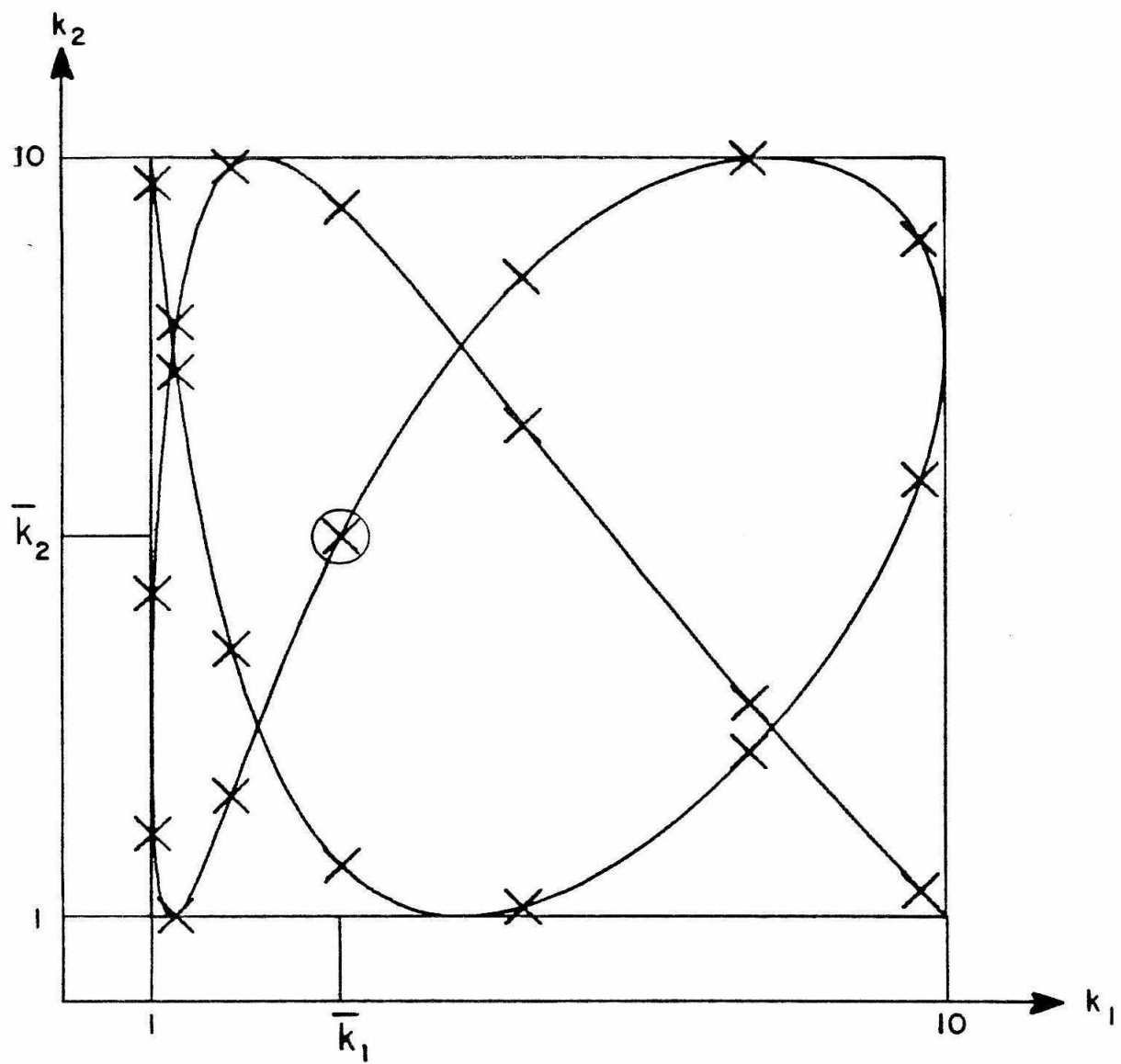


Figure 3. Monte Carlo Approach to Generating the Solution Surface (after Gelinas and Vajk, 1978)

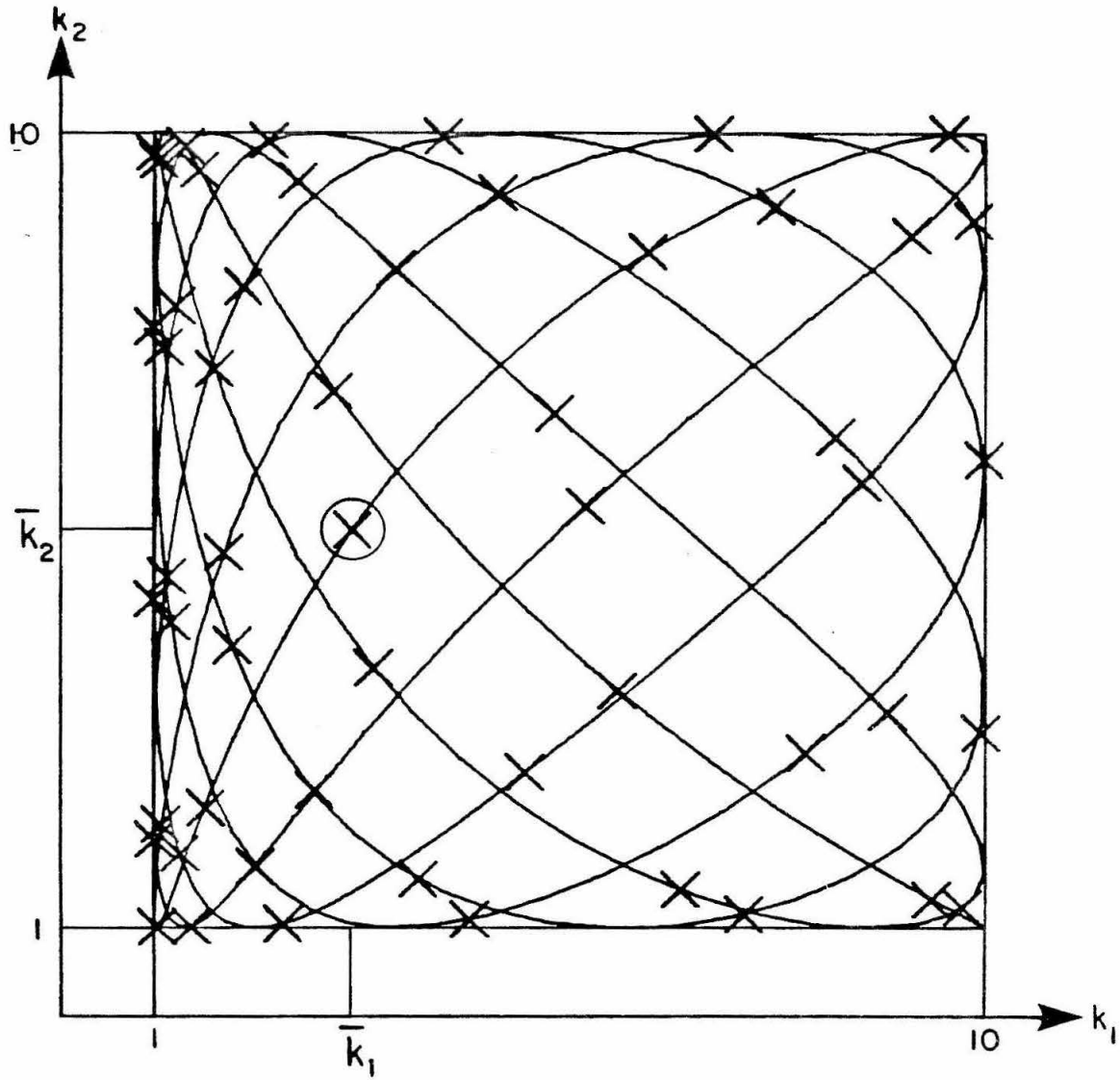


$$k_1 = \bar{k}_1 \exp[\bar{v}_1 \sin(\omega_1 s)]$$

$$k_2 = \bar{k}_2 [1 + \bar{v}_2 \sin(\omega_2 s)]$$

$$\{\omega\} = [3, 5] \quad N = 21$$

Figure 4. Space Filling Search Curve with Frequencies  $\omega_1 = 3$ ,  
 $\omega_2 = 5$



$$k_1 = \bar{k}_1 \exp[\bar{v}_1 \sin(\omega_1 s)]$$

$$k_2 = \bar{k}_2 [1 + \bar{v}_2 \sin(\omega_2 s)]$$

$$\omega = [11, 13] \quad N = 53$$

Figure 5. Space Filling Search Curve with Frequencies  $\omega_1 = 11$ ,  
 $\omega_2 = 13$ .

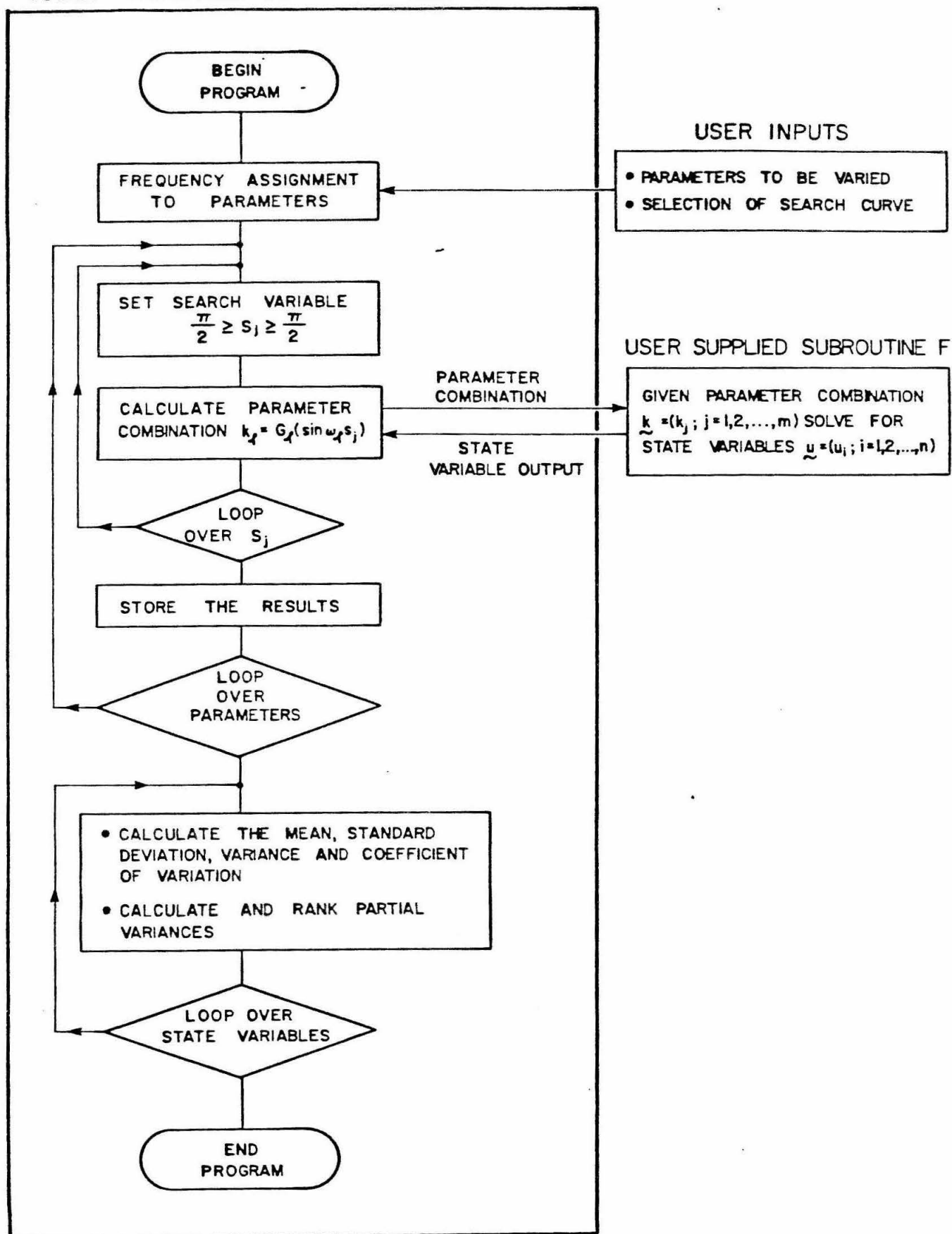


Figure 6. Fourier Amplitude Sensitivity Test Program

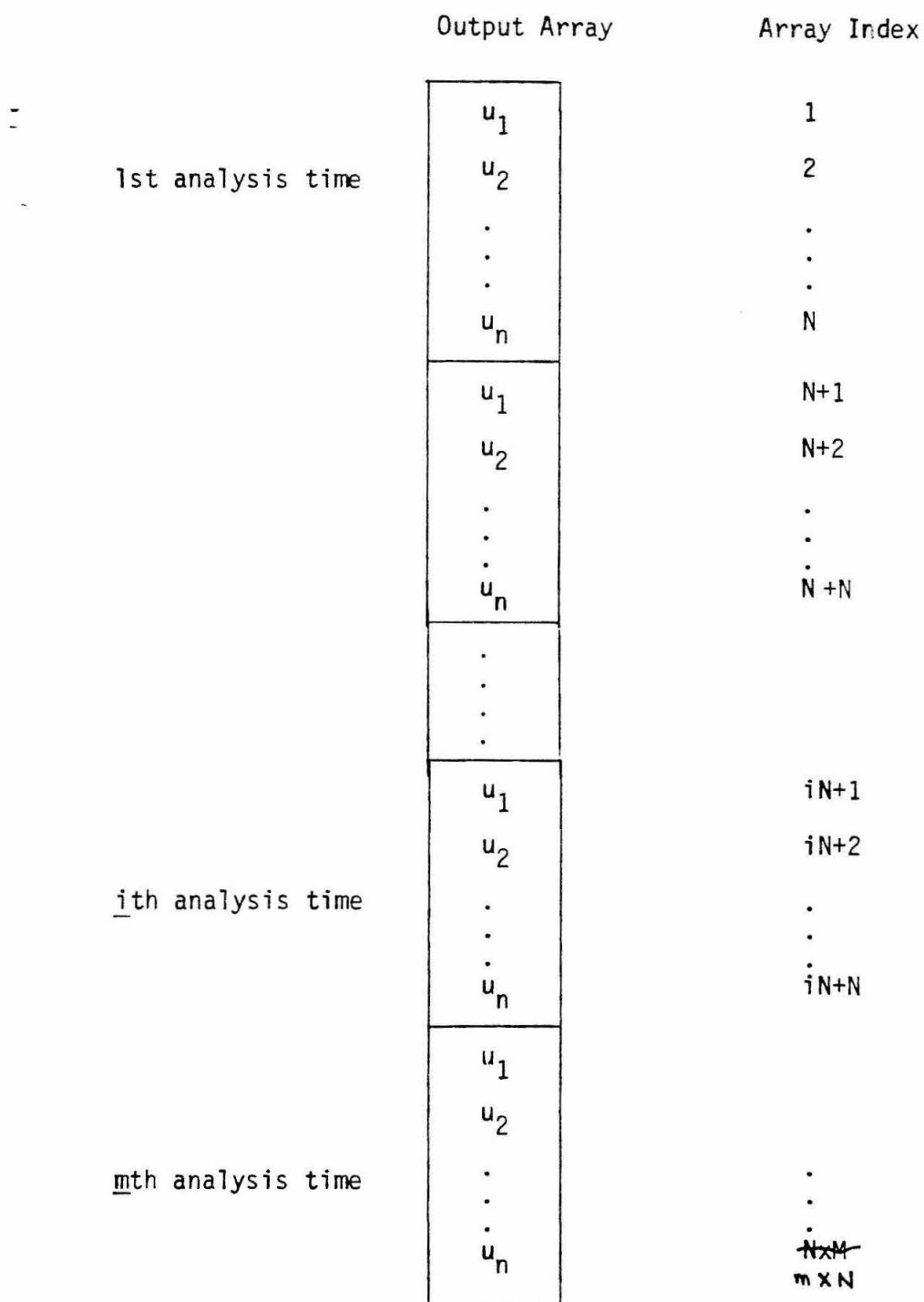


Figure 7. Structure of the Output Array C



SUBROUTINE F(NT,TIME,NPC,NPARM,NSTAT,C)

```

C
- C
- C
C INPUT VARIABLE DESCRIPTION VARIABLE TYPE
C
C NT Number of analysis times Integer
C TIME Array of analysis times Real array
C NPC Current parameter Integer
C Combination number
C NPARM Number of parameters Integer
C P Array of Parameter Values Real Array
C
C OUTPUT VARIABLE DESCRIPTION VARIABLE TYPE
C
C NSTAT Number of output variables Integer
C C Array of state variable values Real array
C Values for each analysis time
C
C DIMENSION TIME (NT), P(NPC), C(1)
C
C F for test problem  $A + X = 2X$ 
C
C DIMENSION P(NPARM),C(1), TIME(NT), S(2)
C
C Unload the parameters
C
C X0=P(1)
C A0=P(2)
C A =P(3)
C B =P(4)
C TA=P(5)
C
C Solve the system
C
C NSTAT=1
C DO 10 J=1,NT
C
C T=TIME (J)
C
C RATE =  $A * \exp(-B/TA)$ 
C
C  $S(1) = 1.0 /$ 
C  $( 1 + (1 - X0) * \exp(-RATE * A0 * T) / X0 )$ 
C
C Store the solution in the proper array
C
C IND=(J-1)*NSTAT
C C(IND+1)=S(1)
10 CONTINUE
C
C RETURN
C END

```

Figure 8. Description of Subroutine F

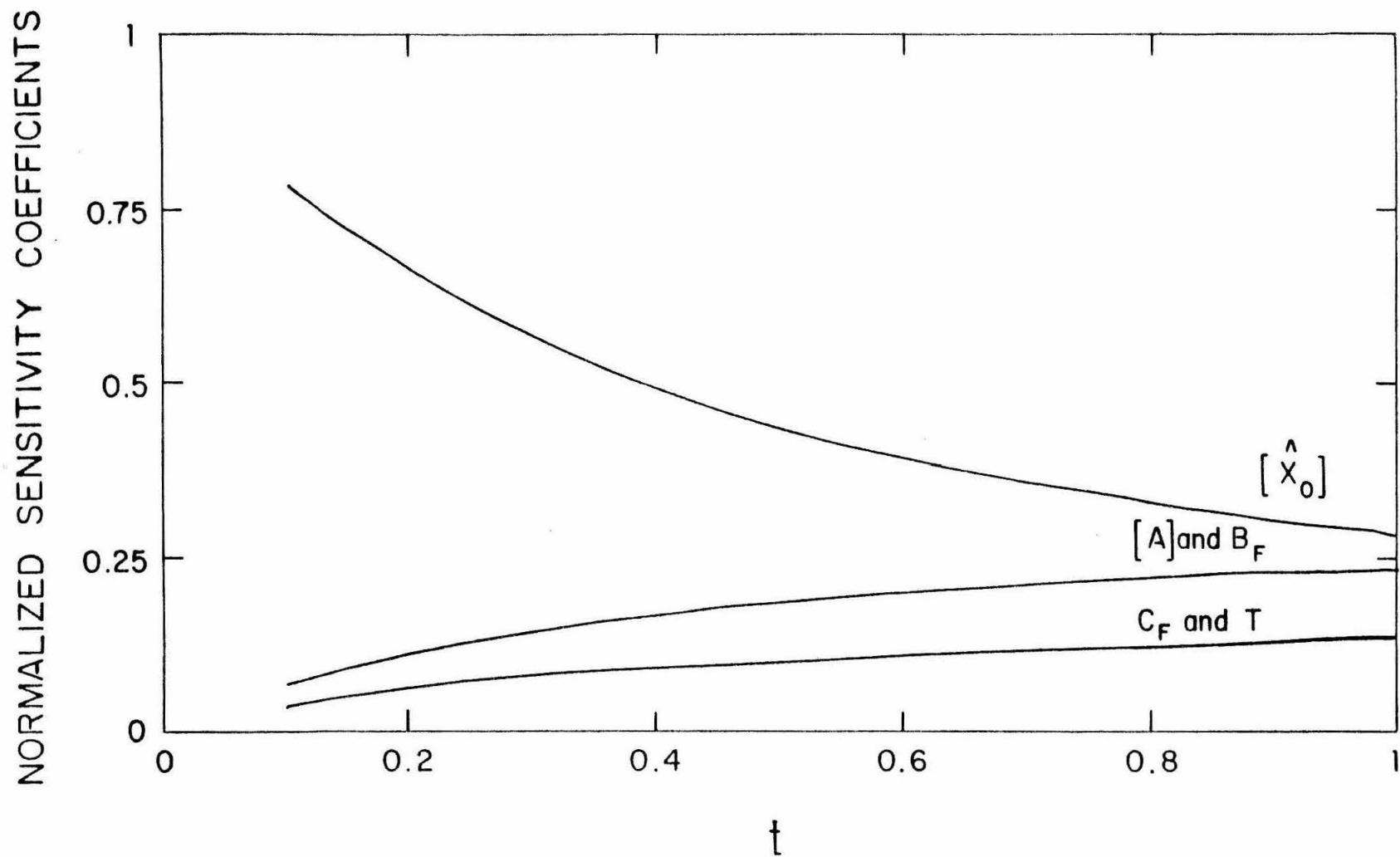


Figure 9. First-Order Sensitivity Coefficients for the Reaction  $A + X \rightleftharpoons 2X$

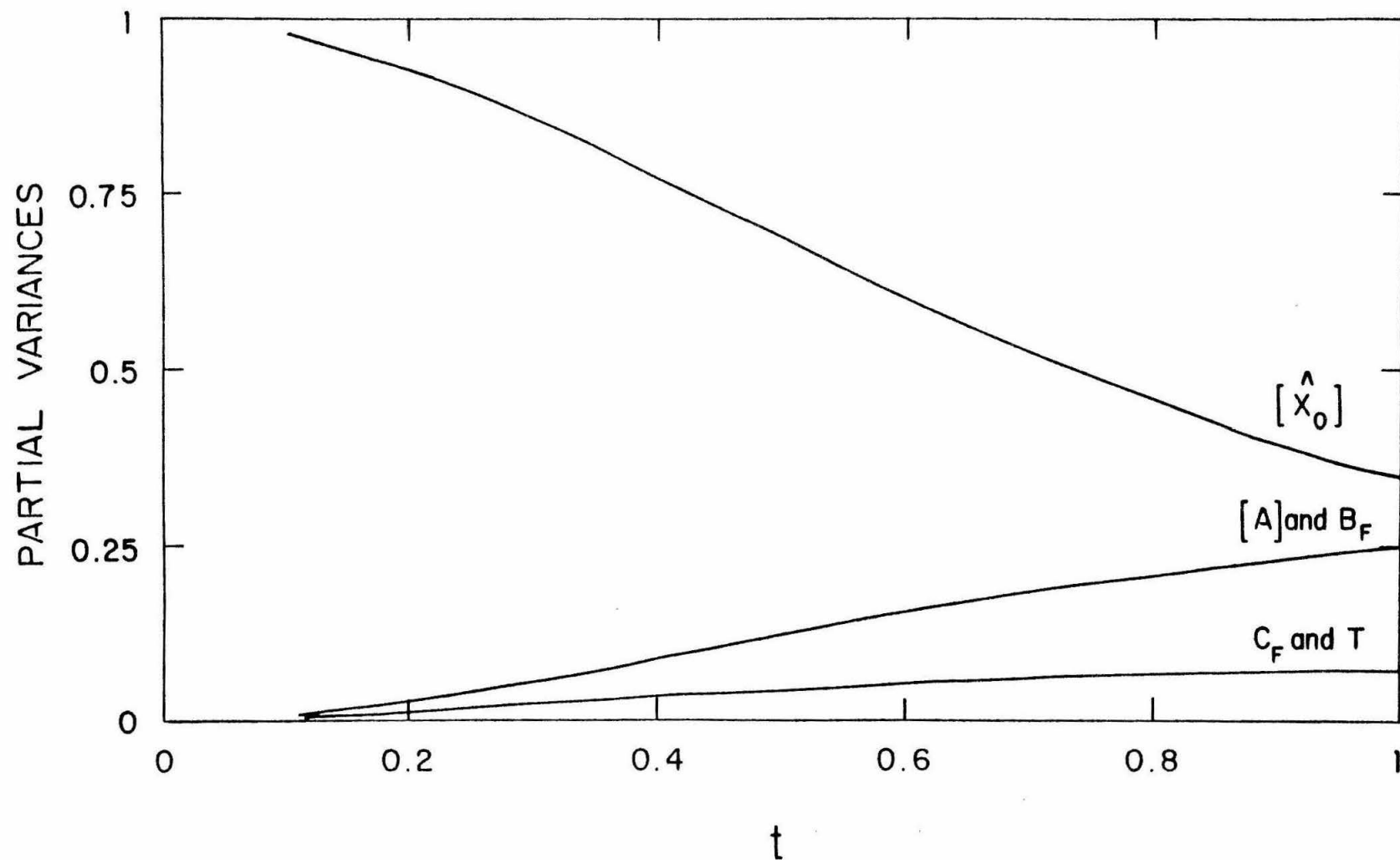


Figure 10. Partial Variances from the FAST Method for the Reaction  $A + X \rightleftharpoons 2X$