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Analysis of Injection-Backflow Tracer Tests

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ABSTRACT

Tracer tests have been an important technique for determining the flaw and reservoir characteristics in various rock matrix systems. While the interwell tracer tests are aimed at the characterization of the regions between the wells, single-well injection-backflow tracer tests may be useful tools of preliminary evaluation, before implementing long term interwell tracer tests.

This work is concerned with the quantitative evaluation of the tracer return profiles obtained from single well injection-backflow tracer tests. First, two mathematical models of tracer transport through fractures, have been reviewed. These two model are based on two different principles: Taylor Dispersion along the fracture and simultaneous diffusion in and out of the adjacent matrix. Then the governing equations for the transport during the injection backflow tests have been solved. Finally the results were applied to field data obtained from Raft River and East Mesa geothermal fields. In order to determine the values of the parameters of the models that define the transport mechanisms through fractures a nonlinear optimization technique was employed.

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1: INTRODUCTION

Reinjection of waste hot water has been commonly practiced in many geothermal reservoirs either as a means of disposal or as a way to maintain the reservoir pressure and liquid volume. In some cases, however, it has been observed that the process had detrimental effects such as early breakthrough of the injected fluids and reduction in the enthalpy.

Since both beneficial and detrimental effects are possible, for the design of a successful reinjection program, the mechanisms of the fluid flow in the reservoir have to be understood. Tracer tests have been an important technique for studying the flow mechanisms in the reservoirs. The quantitative analysis of the test results is possible from studies of the mixing curves by using mathematical models describing the transport mechanism in the reservoir.

As far as the flow of tracer through porous media is concerned, a fairly large number of research results have been published. The models developed for the porous media flow, however, are not necessarily applicable to geothermal reservoirs which are usually highly fractured in nature. In search of a description of the tracer transport mechanisms in fractured reservoirs, so far two basic models have been developed. The first model is the convection-dispersion model which is based on purely dispersive flow through the fracture and the second one is the matrix diffusion model which describes a convective flow in the fracture with simultaneous diffusion into the adjacent matrix. Researchers have used both models in the analysis of the return profiles of interwell tracer tests conducted at different geothermal fields.

So far, interwell tracer tests have been a useful technique in determination of the interconnections between the injectors and the producers. The single well (injection-backflow) tests, on the other hand, have been proposed as tools for characterizing the flow field within the radius of influence around the injectors. Even though the injection backflow tests are proposed as preliminary evaluation tools before the employment of long term interwell tests, the

amount of information that can be recovered from these tests is potentially as much as can be obtained from interwell tests.

In this work, a theoretical study of the return profiles from injection-backflow tracer tests is presented. Both convection-dispersion and matrix diffusion models are employed in the analysis of the return profiles of both continuous injection and spike injection cases. In addition the theoretical results of the continuous injection case are applied to the field data from Raft River and East Mesa geothermal fields by using a nonlinear least squares optimization technique, in order to determine the effective parameters of the tracer transport.

2: LITERATURE SURVEY

Tracer tests have been an important technique for the analysis of the flow mechanisms in various rock matrix systems. The quantitative analysis of the test results is possible through the use of mathematical models describing the tracer transport mechanisms in reservoirs. As far as the flow through porous media is concerned the theory is well established.

Johnston and Perkins (1963) summarized the dispersion in porous media and gave the empirical correlations to determine the parameters of the classic convection- dispersion model.

In 1964, *Coats and Smith* modified the one-dimensional convection-dispersion model to obtain a differential capacitance model which allows mass transfer between the mobile and immobile fractions of the liquid phase in the reservoir. With the differential capacitance model they were able to produce the asymmetric concentration profiles observed from the experiments. Later in 1976, *van Genuchten and Wierenga,* improved the model by including a term for the adsorption taking place in both mobile and immobile regions.

However, the models developed to describe the tracer transport mechanisms in porous media are not applicable to highly fractured geothermal reservoirs. Recent studies on flow through fractured media, led to the development of new models describing the physics of the tracer transport through fractures.

Grisuk and Pickens (1980) formulated a double porosity model combining a convective-dispersive transport the in fractures and a diffusive transport in the unfractured matrix. A finite element method was developed for simulating non-reactive and reactive solute transport by convection, mechanical dispersion and diffusion in a unidirectional flow field.

In 1981, *Rodriguez and Horne* presented a theoretical study of the one-dimensional convective-dispersive flow through fractures. In that work, they derived an expression for for the dispersivity in flow through a fracture. *Fossum and Horne* (1982) applied this model to in-

terwell tracer test data obtained from Wairakei, New Zealand with some success. They used a nonlinear optimization technique to perform matching the model to field data.

In 1982, from the studies of migration of radionuclides in bedrock surrounding,nuclear waste repositories, ***Neretnieks, Eriksen and Tahtinen*** developed a matrix diffusion model describing the tracer movement in a single fissure in granitic rock. Using this matrix diffusion model ***Jensen and Horne*** (1983) were able to obtain a better match model to the data obtained from Wairakei, New Zealand as compared to the dispersion model used by Fossum and Horne (1982).

Walkup and Horne (1985) developed a *two* dimensional model which uses the tracer loss terms of the matrix diffusion model and at the same time allows the direct determination of the fracture aperture. Even though matching to field data with nonlinear curve fitting was suecessful, excessive computer time consumption was a serious limitation,

Single well tracer tests have been used to estimate the immobile fluid saturation to determine the waterflood conformance and to evaluate the potential of chemical enhanced oil recovery processes by the oil and gas industry. Recently ***Antunez and Brigham*** (1983), developed a semi-analytical method to analyze the single well tests in oil reservoirs and presented a set of charts for the estimation of residual oil saturation.

Unlike in oil reservoirs, the use of the single well tracer tests in geothermal reservoirs has started only recently. The interwell tracer tests have been commonly practised to determine the interconnections between the injectors and producers and to characterize the reservoir flow mechanisms. In these interwell tests it has been observed that the tracer breakthrough does not always occur within the expected times. It was also found that the tracers could be physically and chemically restrained by the reservoir matrix rocks or the fluid could be moving through locations where there are no monitor wells. For these reasons the single well (injection-backflow) tracer tests have been proposed as a preliminary evaluation technique before the implementation of the long term interwell tests.

In 1982, *Downs* and his coworkers presented a preliminary study of the injection-backflow tests conducted at Raft River Geothermal Field. Later in **1983,** *Capuano* ***et al.*** presented the qualitative analysis of the **tests** conducted at both Raft River and East Mesa fields. It was concluded that the injection-backflow tracer **tests** can **be** successfully **used** to characterize the flow in the near well-bore environment. In another study of the same tests, Russel et *al.* analyzed the tracer return profiles by using the semi-infinite medium solution to the one-dimensional convection-dispersion model.

3: THEORY

Tracer tests have been important tools for the study of the flow mechanisms in geothermal reservoirs. In interwell tests a tracer fluid of constant concentration is injected into the reservoir at one well and the tracer is monitored at other wells. If the fluid arrives at the monitor location then inferences can be made about the reservoir flow conditions between the two wells. The most direct information about the interconnection between the injection and observation wells is obtained from the mean arrival times. Also, from the shape of the return profiles, the dispersive characteristics can be analyzed. If the arrival times are longer than expected, the fluid could be physically and chemically restrained by the matrix rocks, it could be moving through locations where there are no monitor wells, or it could be dispersing in an orderly manner.

In a reference prepared by the University of Utah Research Institute Earth Sciences Laboratory, injection-backflow tests have been proposed as a preliminary evaluation technique before the implementation of the long term interwell tests. In the report the following advantages of the injection-backflow tests were listed:

a) A suite of tracers can be easily evaluated and those which interact with the formation can be eliminated and conservative tracers can be established.

b) With the conservative tracer established, the mixing of the injected fluid with the reservoir fluid can be studied. From the analysis of the mixing curves selected reservoir characteristics can be determined.

c) If the injected fluid moves from an area of fractures into a porous matrix or vice versa during the injection flow this may be detectable as a discontinuity in the tracer return flow.

d) The chemical reactions between the injected fluid and rock matrix and native fluid can be assessed by analyzing the injected and returning fluids.

e) Deposition of the fluids can be assessed by analyzing the solid particles in the injected and returning fluids.

f) With the temperature of the injected and returning fluids known, together the mixing of the injected and native fluids and the time in the formation, the heat transfer may be related to matrix porosity.

g) Regional reservoir flow in the area of the injection well can be assessed by delaying the backflow from the test well. Loss of tracer would indicate a substantial flow in the reservoir with the tracer moving beyond the well's radius of influence.

The injection backflow tests can be divided into three stages : a) Injection period , b) Shut-in period, c) Backflow period. However, if the test is not aimed at the determination of regional flow beyond the test well's radius of influence, it may be completed in only two stages, injection and immediate backflowing.

Since the transport of tracers through geothermal reservoirs is primarily through fractures, the success of interpretive analysis of the return curves depends on the understanding the physics of the mixing process during the flow. In this work, two mathematical models based on two principal mechanisms, dispersion in fracture and the diffusion into the matrix, were employed to analyze the tracer return profiles from injection and immediate backflowing tests.

The injection-backflow tests can be conducted either injecting a tracer fluid of concentration C_o continuously during the injection period (continuous injection case) or injecting a tracer slug followed by the untraced fluid (slug or spike injection case depending upon the size of the slug). Here, both continuous injection and spike injection cases for both convection-dispersion and matrix diffusion models will be considered.

3.1 CONVECTION-DISPERSION MODEL

In a fracture, under either laminar or turbulent flow the fluid will be transported faster in the center of the fracture than near the walls. The result of this non-uniform "convective" transport is the dispersion of the tracer over the region of the transport. Although this convective smearing of the tracer gives rise to large concentration gradients across the narrow width of the fracture, molecular diffusion tends to rapidly equalize the tracer concentration across the fracture, thus counteracting the effect of convective dispersion.

The combination of the transverse diffusion and convective dispersion in the flow channel is known as "Taylor Dispersion" and was derived by Taylor (1953) for pipe flow. **The net result of The Taylor Dispersion is that the tracer front propagates with the mean speed of the flow.** The net longitudinal dispersivity for the the combination is :

$$\eta = \frac{2}{105}\frac{b^2u^2}{D} \tag{3.1}$$

where

b : the fracture aperture

u : the average velocity

D : the molecular diffusion coefficient

as derived by Home and Rodriguez (1983).

Taylor (1953) presents the equation governing the effective longitudinal dispersion in an infinite medium

$$\eta \frac{\partial^2 C}{\partial z^2} = \frac{\partial C}{\partial t} \tag{3.2}$$

where

$$z = x - ut$$

x : distance

u : average velocity

t : time

C : concentration

η : Taylor dispersion coefficient

3.1.1 Continuous Injection Case

For the continuous injection case the boundary and initial conditions are

$$C = 0 \qquad at \quad t = 0$$
$$C = C_o \qquad at \quad z = -\infty$$
$$C = 0 \qquad at \quad z = \infty$$

The solution to Eq.3.2 with the above boundary and initial conditions is given by Taylor

$$\frac{C}{C_o} = C_D = \frac{1}{2} erfc\left[\frac{x - ut}{2\sqrt{\eta t}}\right] \tag{3.3}$$

Eq. 3.3 represents the concentration profile during the injection period and it is symmetric about $x = ut$ which is the average distance traveled by the front. Alsd the point $x = ut$ corresponds to position of the 50 percent concentration contour. If L_t is the zone of transition in which C_D changes from 0.9 C_D to 0.1 C_D , the expression for L_t , is given by Taylor

$$L_t = 3.62\sqrt{\eta t}$$

Taylor also mentioned that as t increases L, increase proportionally to $t^{\frac{1}{2}}$ whereas the distance traveled by the particles of fluid are proportional to t. Eventually as t increases L_t become small compared with L = ut which is the distance traveled by the moving plane traveling with the mean speed of flow, u. Therefore there is a minimum injection time requirement for the theory to be applicable. At the end of the injection period of time t_j, the profile is given by

$$\frac{C}{C_o} = \frac{1}{2} erfc\left[\frac{x - utj}{2\sqrt{\eta t_j}}\right] \tag{3.4}$$

The analysis of the injection backflow tests is not a simple one-dimensional problem, because of the change in flow direction during the backflow period. There is also a possibility of change in the average flow velocity during the backflow period. For these reasons, to obtain the backflow period profile the governing equations have to be solved with appropriate initial and boundary conditions. However, for this specific problem, here we will apply a simpler technique developed by Antunez and Brigham (1983), to obtain the solutions.

In this case, first with the assumption of equal average flow velocities during injection and backflow periods, the problem is simplified. From Eq. 3.4 the concentration profile at the and of the injection period is given by Fig. 3.1

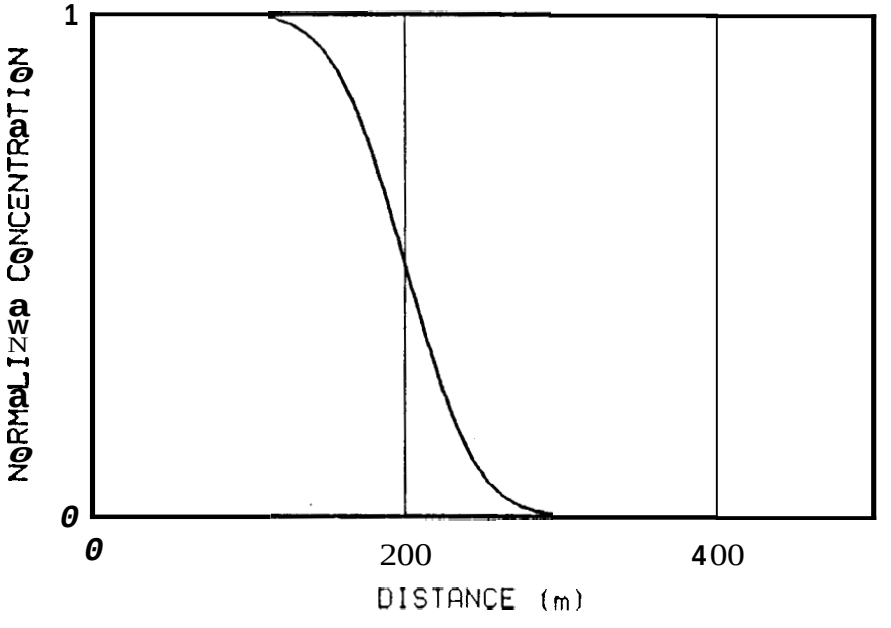

Fig. 3.1 Dispersion of a Sharp interface Caused by Taylor Dispersion.

The 50 percent concentration point is at a distance of $x = L$ to the injection point $x = 0$, and the profile is symmetric about this point. At this point, first of all, we have to remember

that the front propagates with the mean speed of the flow. To obtain the backflow period solution we utilize both the equal injection and backflow average velocities and the symmetry of the profile. During the backflow period we imagine a pseudo-front going away from the injection point as if the injection period is continuing, while the real front approaches the well. Since the injection and backfiow velocities are imagined to be equal for both real and pseudo fronts, the distance traveled by them will also be equal. The schematics of the process is given in Fig. 3.2

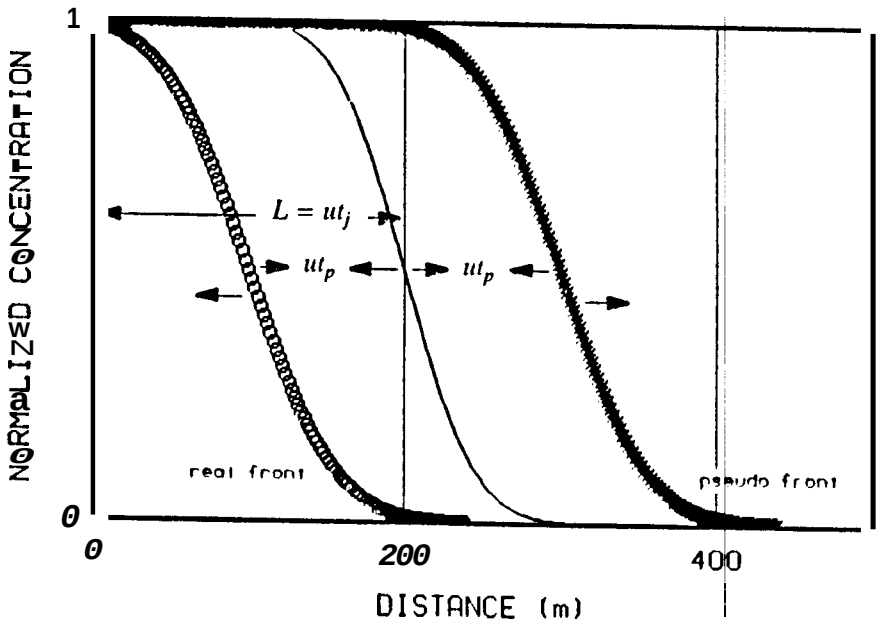

Fig. 3.2 Positions of Real and Pseudo Fronts.

Then the concentration of the pseudo-profile at any distance x is given by

$$\frac{C_p}{C_o} = \frac{1}{2} erfc\left[\frac{x - u(t_j + t_p)}{2\sqrt{\eta(t_j + t_p)}}\right] \tag{3.5}$$

If the concentrations of the pseudo-profile were to be calculated at $x = 2L = 2ut_j$, then

$$\frac{C_p}{C_o} = \frac{1}{2} erfc\left\{\frac{u(t_j - t_p)}{2\sqrt{\eta(t_j + t_p)}}\right\} \tag{3.6}$$

When the 50 percent concentration of the pseudo-front reaches to $x = 2L$, the same concentration of the real front reaches to well which is the measurement point. Therefore, the concentrations measured at the well can be calculated by using the pseudo-front concentrations evaluated at $x = 2L$. The pseudo concentration C_p is related to the actual concentration C_r by

$$\frac{C_r}{C_o} = 1 - \frac{C_p}{C_o} = 1 - \frac{1}{2} erfc\left\{\frac{u(t_j - t_p)}{2\sqrt{\eta(t_j + t_p)}}\right\} \tag{3.7}$$

Therefore

$$\frac{C_r}{C_o} = \frac{1}{2} + \frac{1}{2} erf\left\{\frac{u(t_j - t_p)}{2\sqrt{\eta(t_j + t_p)}}\right\} \tag{3.8}$$

where

t_j : injection time

t_p : production time

u : the average velocity

η : the dispersion coefficient

Defining $a = \frac{u}{\sqrt{\eta}}$ and $C_D = \frac{C_r}{C_o}$ Eq.3.8 can be rewritten as

$$C_D = \frac{1}{2} + \frac{1}{2} erf\left[\frac{\alpha(t_j + t_p)}{2\sqrt{t_j + t_p}}\right] \tag{3.9}$$

3.1.2 Spike Injection Case

In tracer studies, it is more common to inject small slugs than continuously injaction of the tracer fluid, due to the cost of operation. When a slug is injected into a reservoir the concentration can be expressed as the difference between the two dispersed fronts which are called the leading and the trailing edges. Since the flow of a tracer slug through a fracture is linear one-dimensional flow, the concentration profile can be expressed as,

$$\frac{C}{C_o} = \frac{1}{2} erfc\left[\frac{x - ut_1}{2\sqrt{\eta t_1}}\right] - \frac{1}{2} erfc\left[\frac{x - ut_2}{2\sqrt{\eta t_2}}\right] \tag{3.10}$$

If the size of the slug is very small compared to the distance traveled by it, in the limit the solution can be found as follows. The response to a plane source of unit strength concentrated at $x = x' = ut$ in an infinite medium, is given by the Green's Function Solution,

$$C = \frac{1}{2\sqrt{\pi\eta t}} \; e^{\frac{-(x-ut)^2}{4\eta t}} \tag{3.11}$$

If the source is of strength s (mass/unit area), then the response is

$$C = \frac{S}{2\sqrt{\pi\eta t}} \; e^{\frac{-(x-ut)^2}{4\eta t}} \tag{3.12}$$

The tracers are injected in tracer fluids of a specified concentrations C_o. Then if a volume of $V = AL_1$ tracer fluid is injected, the mass of the tracer is given by

$$M = C_o V = C_o A L_1$$

$$S = \frac{M}{A} = \frac{C_o A L_1}{A} = C_o L_1 \tag{3.13}$$

Finally the concentration distribution is given by

$$\frac{C}{C_o} = \frac{L_1}{2\sqrt{\pi\eta t}} \; e^{\frac{-(x-ut)^2}{4\eta t}} \tag{3.14}$$

where L_1 is the length of the slug.

However, since the fracture dimensions are unknown we do not know the slug length entering the reservoir. Therefore we rewrite Eq.3.14 by using more explicit variables. The total volume of tracer fluid can be represented by

$$V = injection\ rate * time\ of\ injection\ of\ the\ traced\ fluid$$

Then, source strength can be represented as

$$S = \frac{C_o Q\, t_i}{A} = C_o t_i \frac{Q}{A} = C_o t_i u$$

Now, we can rewrite **Eq.3.14** as

$$\frac{C}{C_o} = \frac{ut_i}{2\sqrt{\pi\eta t}} \; e^{\frac{-(x-ut)^2}{4\eta t}} \qquad (3.15)$$

Eq. 3.15 represents the concentration profile during the injection period for the spike injection case. An important feature of **Eq. 3.15** is that it is symmetric about $x = ut$, which corresponds to the peak concentration. To obtain the concentration profile at the end of the injection period the variable **t** in **Eq. 3.15** is replaced by t_j.

$$\frac{C}{C_o} = \frac{ut_i}{2\sqrt{\pi\eta t_j}} \; e^{\frac{-(x-ut_j)^2}{4\eta t_j}} \qquad (3.16)$$

The schematics of the Eq. **3.15** is given in Fig. **3.3**

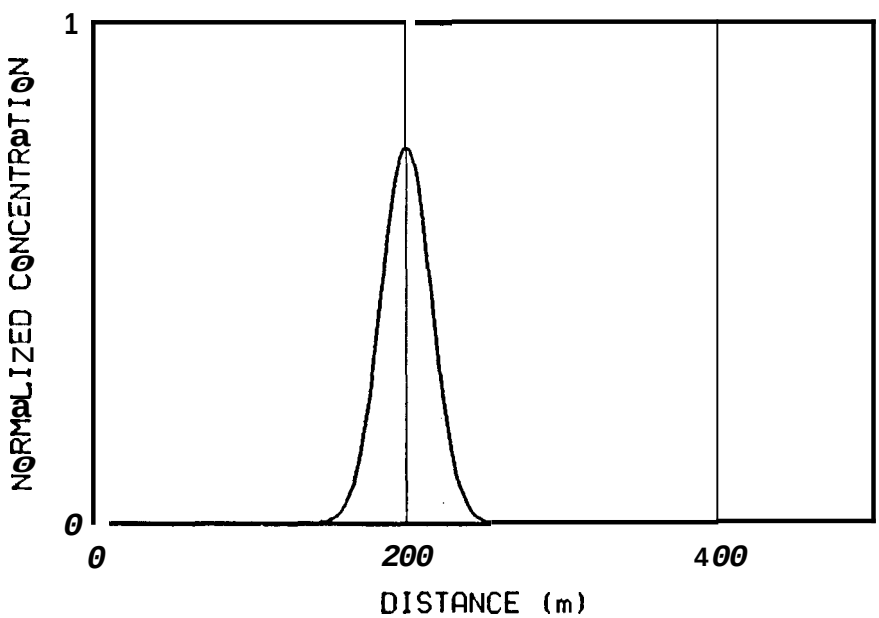

Fig. **3.3** Dispersion *of* **a Slug Caused by Taylor** Dispersion.

The concentrations measured at the well during the backflow period can be calculated as follow. During the backflow period we assume as we did for the continuous injection case- a pseudo-slug going away from the injection point as if the injection process is continuing. Assuming the injection and backflow velocities are equal, the distances traveled by the peak concentrations of real and pseudo slugs will be the same; as it is shown in Fig. 3.4

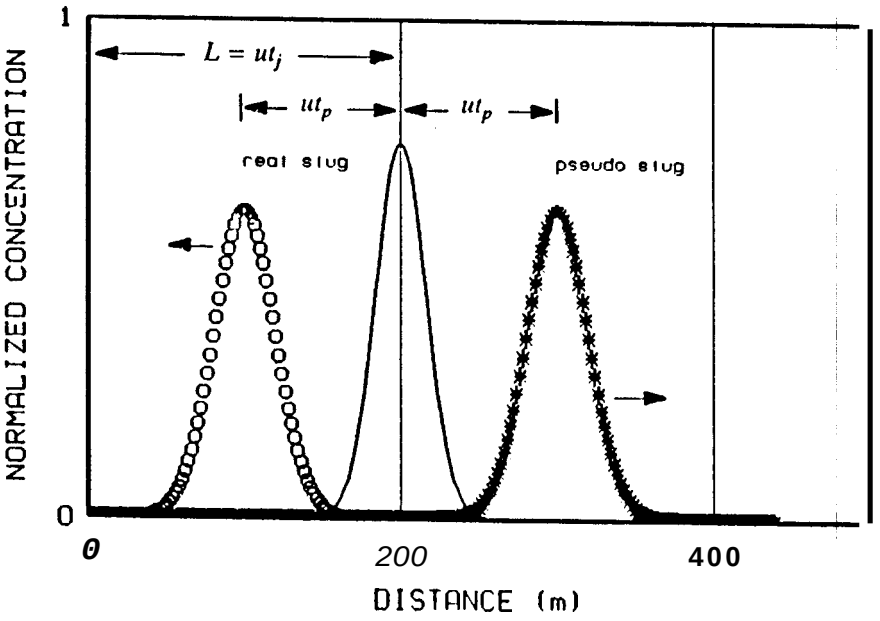

Fig. 3.4 Positions of Real arid Pseudo Slugs.

Then the concentration profile of the pseudo slug at any backflow time is given by

$$\frac{C}{C_o} = \frac{ut_i}{2\sqrt{\pi\eta(t_j + t_p)}}\ e^{\frac{-(x - u(t_j + t_p))^2}{4\eta(t_j + t_p)}} \qquad (3.17)$$

If the distance is set to $x = 2L = 2ut_j$,the expression becomes

$$\frac{C}{C_o} = \frac{ut_i}{2\sqrt{\pi\eta(t_j + t_p)}}\ e^{\frac{-u^2(t_j - t_p)^2}{4\eta(t_j + t_p)}} \qquad (3.18)$$

Since the profiles are symmetric about the peak point concentrations, the calculated values of pseudo slug concentration at $x = 2L$, will be equal exactly to the concentrations measured at the well. Hence, the solution becomes,

$$\frac{C}{C_o} = \frac{ut_i}{2\sqrt{\pi\eta(t_j + t_p)}} \; e^{\frac{-u^2 (t_j - t_p)^2}{4\eta(t_j + t_p)}} \tag{3.19}$$

where

t_j : total injection time

t_p : production time

u : the average velocity

η : the dispersion coefficient

t_i : length of the slug injection time

Defining a new parameter $a = \frac{u}{\sqrt{\eta}}$ and $C_D = \frac{C}{C_o}$, Eq.3.19 becomes

$$C_D = \frac{C}{C_o} = \frac{\alpha t_i}{2\sqrt{\pi(t_j + t_p)}} \; e^{\frac{-\alpha^2 (t_j - t_p)^2}{4(t_j + t_p)}} \tag{3.20}$$

3.2 MATRIX DIFFUSION MODEL

When a tracer fluid flows in a fracture, the tracer will diffuse into the porous matrix adjacent to the fracture. For very large spacing between the fissures, the one-dimensional form of the equation of the diffusion into the porous matrix is given by

$$\frac{\partial}{\partial y}\left[\phi D_a \frac{\partial C_p}{\partial y}\right] = \phi \frac{\partial C_p}{\partial t} \tag{3.21}$$

Assuming the porosity ϕ, and the apparent diffusion coefficient D_a are constant throughout the matrix contacted by the fluid the Eq. 3.21 takes the form,

$$D_a \frac{\partial^2 C_p}{\partial y^2} = \frac{\partial C_p}{\partial t} \qquad (3.22)$$

When the source of the tracer fluid is discontinued the effect will be to flush the fracture and reverse the concentration gradient causing tracer to migrate from the matrix into the fracture.

Assuming the concentration profile across the fracture is evened out due to molecular diffusion, the flow and sorption from the water in fracture is represented by

$$\frac{\partial C_f}{\text{at}} + u \frac{\partial C_f}{\partial x} = 2\frac{D_e}{\delta} \frac{\partial C_r}{\partial y}\Big|_{y=0}$$

The two diffusion coefficients D, and D_e in Eq. 3.22 and 3.23 respectively, are related as follow:

$$D_a = \frac{D_e}{K_d \rho_b} \qquad (3.24)$$

The effective diffusion coefficient D_e, is dependent on temperature, porosity, molecular diffusivity and the geometry of the rock. $K_d\rho_b$ is a volumetric sorption equilibrium constant, and is related to porosity ϕ, the solid rock density ρ_s and the adsorption distribution coefficient k by,

$$K_d \rho_b = \phi + (1 - \phi)k\rho_s \qquad (3.25)$$

If the solids are inert, i.e $k = 0$ which we assumed in this work, the volumetric sorption equilibrium constant of the mamx becomes equal to its porosity. Then, the Eq.3.25 reduces to

$$D_a = \frac{D_e}{\phi} \qquad (3.26)$$

Equations 3.22 and 3.23 are the system of equations describing the physical situation of one-dimensional convective flow through a fracture with simultaneous tracer diffusion into the surrounding porous matrix. To be able to determine the concentration profile\$, Equations 3.22 and 3.23 have to be solved simultaneously. Here the solutions for both continuous injection and spike injection cases will be presented.

3.2.1 Continuous Injection Case

For a constant solute source of C_o at $x = 0$, initially the media are saturated with fluids free from the tracer, the boundary and initial conditions are given as,

$$C_f = C_p = 0 \qquad at \qquad t = 0$$

$$C_f = C_0 \qquad at \qquad x = 0$$

$$C_p = C_f \qquad at \qquad y = 0$$

$$C_p \to 0 \qquad as \qquad y \to \infty$$

If we assume $C_o = 1$ then the solutions we will obtain will be in terms of normalized concentrations. By using the Laplace transform method, we obtain the solution in Laplace space

$$\overline{C_f} = \frac{1}{s} \; e^{-\frac{x}{u}s} \; e^{\frac{-2\sqrt{D_e\phi}}{\delta u}x\sqrt{s}} \tag{3.27}$$

$$\overline{C_p} = \frac{1}{s} \; e^{-\frac{x}{u}s} \; e^{-\left[\frac{2\sqrt{D_e\phi}\,x}{\delta u} + \sqrt{\frac{\phi}{D_e}}\,y\right]\sqrt{s}} \tag{3.28}$$

where s is the Laplace parameter, and Equations **3.26** and **3.27** are the solutions in Laplace space for the concentrations in fracture and porous matrix respectively.

The solutions in real space are

$$C_f = erfc\left[\frac{\sqrt{D_e\phi}}{\delta}\frac{x}{u}\frac{1}{\sqrt{t - \frac{x}{u}}}\right] \qquad \text{for} \quad t > \frac{x}{u} \tag{3.28}$$

$$C_p = erfc\left\{\left[2\frac{\sqrt{D_e\phi}}{\delta}\frac{x}{u} + \sqrt{\frac{\phi}{D_e}}y\right]\frac{1}{2\sqrt{t-\frac{x}{u}}}\right\} \qquad \text{for} \quad t > \frac{x}{u} \tag{3.29}$$

and both C_f and C_p are zero for $t < \frac{x}{u}$.

Equations **3.28** and **3.29** represent the injection period concentration profiles in the fracture and in the porous matrix respectively. At the end of the injection period of time t_j, the solutions are,

$$C_f = erfc\left[\frac{\sqrt{D_e\phi}}{\delta}\frac{x}{u}\frac{1}{\sqrt{t_j-\frac{x}{u}}}\right] \qquad \text{for} \quad t_j \geq \frac{x}{u} \tag{3.30}$$

and

$$C_f = 0 \qquad \text{for} \quad t_j < \frac{x}{u}$$

$$C_p = erfc\left\{\left[2\frac{\sqrt{D_e\phi}}{\delta}\frac{x}{u} + \sqrt{\frac{\phi}{D_e}}y\right]\frac{1}{2\sqrt{t_j-\frac{x}{u}}}\right\} \qquad \text{for} \quad t_j \geq \frac{x}{u} \tag{3.31}$$

and

$$C_p = 0 \qquad \text{for} \quad t_j < \frac{x}{u}$$

Since the flow direction changes, the backflow period concentrations have to be obtained by solving the governing system of equations with appropriate initial and boundary conditions.

The injection period profile in the fracture will be as in Fig. **3.5**

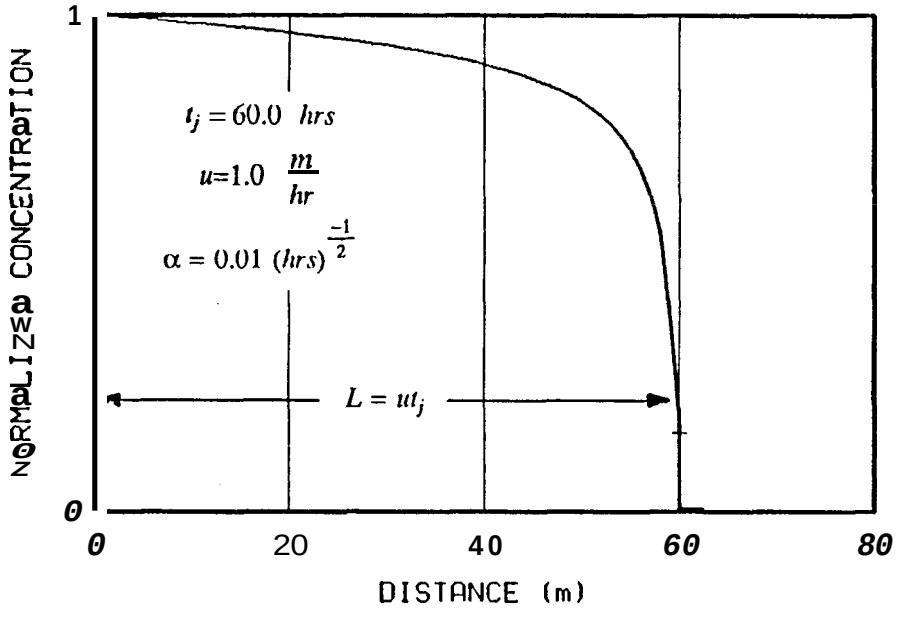

Fig. 3.5 Dispersion **of a** Sharp Interface Caused **by Matrix** Diffusion.

In the backflow period, to take the change in the direction of the velocity vector into account, the governing differential equations have to be modified. Here the modification will be done by utilizing the nature of the injection period solution and making a simple coordinate change.

Looking at the profile at the end of the injection period it is seen that the concentration in the fracture is zero after a distance of $x = ut_j = L$, as seen from Fig. **3.5** When the origin of the new coordinate system is chosen at $x = L$ and the new space variable is defined as z, the injection period profile can be expressed in terms of z, by simply replacing **x** by $L - z$.

$$C_f = erfc\left[\frac{\sqrt{D_e\phi}}{\delta}\,\frac{L-z}{u}\,\frac{1}{\sqrt{t_j - \frac{L-z}{u}}}\right] \qquad \text{for} \quad t_j \geq \frac{L-z}{u} \tag{3.32}$$

$$C_f = 0 \qquad \text{for} \quad t_j < \frac{L-z}{u}$$

$$C_p = erfc\left\{\left[\frac{2\sqrt{D_e\phi}}{\delta}\,\frac{L-z}{u} + \sqrt{\frac{\phi}{D_e}}\,y\right]\frac{1}{2\sqrt{t_j - \frac{L-z}{u}}}\right\}$$

$$\text{for} \quad t_j \geq \frac{L-z}{u} \tag{3.33}$$

$$C_p = 0 \qquad \text{for} \quad t_j < \frac{L-z}{u}$$

Now with the new coordinate system, the governing differential equation of flow in the fracture becomes

$$\frac{\partial C_f}{\partial \tau} + u\,\frac{\partial C_f}{\partial z} = \frac{2D_e}{\delta}\,\frac{\partial C_p}{\partial y}\bigg|_{y=0} \tag{3.34}$$

where τ is the time coordinate, starting from the beginning of the backflow period.

As far as the diffusion of tracer into or out of the matrix is concerned, there is no change in the conditions for constructing the governing equation. Hence, the equation remains the same.

$$D_a\frac{\partial^2 C_p}{\partial y^2} = \frac{\partial C_p}{\partial \tau} \tag{3.35}$$

the boundary conditions are

$C_f = 0$ at $z = 0$ $\tau \geq 0$

$C_p = C_f$ at $y = o$ $\tau \geq 0$

$C_p \to \infty$ as $y \to \infty$ $\tau \geq 0$

and the initial conditions are

$$C_f = erfc\left\{\frac{\sqrt{D_e\phi}}{\delta}\,\frac{L-z}{u}\,\frac{1}{\sqrt{t_j - \frac{L-z}{u}}}\right\} \tag{3.36}$$

$$at \quad \tau = 0 \quad \text{and} \quad 0 \le z \le L$$

$$C_p = erfc\left\{\left[2\frac{\sqrt{D_e\phi}}{\delta}\,\frac{L-z}{u} + \sqrt{\frac{\Phi}{D_e}}y\right]\frac{1}{2\sqrt{t_j - \frac{L-z}{u}}}\right\} \tag{3.37}$$

$$at \quad \tau = 0 \quad \text{and} \quad 0 \le z \le L$$

However, the attempts to obtain the real space solutions to Equations 3.34 and 3.35 failed because of the complexity induced by the initial conditions. For this reason, the Laplace transformed forms of the initial conditions will be preserved, and a solution in Laplace space will be obtained.

The initial conditions in Laplace space are

$$\bar{C}_f = \frac{1}{s}e^{-\frac{x}{u}s}\,e^{\frac{-2\sqrt{D_e\phi}}{\delta u}x\sqrt{s}} \tag{3.38}$$

$$\bar{C}_p = \frac{1}{s}e^{-\frac{x}{u}s}\,e^{-\left[\frac{2\sqrt{D_e\phi}}{\delta}\frac{x}{u} + \sqrt{\frac{\Phi}{D_e}}y\right]\sqrt{s}} \tag{3.39}$$

where s is the Laplace parameter corresponding to time $t = t_j$

Now the initial conditions are given by Equations 3.38 and 3.39. When we take the Laplace transform of Eq. 3.35 according to the time variable, τ,

$$\frac{\partial^2\tilde{C}_p(z,s,p)}{\partial y^2} - \frac{p}{D_a}\tilde{C}_f(z,s,p) = -\frac{1}{s\,D_a}e^{-\beta\sqrt{s}}\,e^{-xs/u}e^{-\sqrt{\frac{s}{D_a}}y} \tag{3.40}$$

where $\beta = \frac{2\sqrt{D_e \phi}\, x}{\delta u}$ and p is the Laplace parameter corresponding to time τ. The result is a linear nonhomogeneous differential equation and the solution is given **by**

$$\bar{C}_p(z,s,p) = \bar{C}_f(z,s,p)\, e^{-\sqrt{\frac{p}{D_a}}y} - e^{-xs/u}\, \frac{e^{-\beta\sqrt{s}}}{(p-s)}\left[e^{-\sqrt{\frac{p}{D_a}}y} - e^{-\sqrt{\frac{s}{D_a}}y}\right] \tag{3.41}$$

using the property that the transform of the derivative of a function is equal to the derivative of the transform of the function in Laplace space,

$$L\left\{\left[\frac{\partial C_p}{\partial y}\right]_{y=0}\right\} = \left\{\left[\frac{\partial \bar{C}_p}{\partial y}\right]_{y=0}\right\} \tag{3.42}$$

The Laplace transform of the Eq. **3.34** can **be** written as

$$p\bar{C}_f(z,s,p) - \bar{C}_f(z,s) + u\frac{\partial \bar{C}_f(z,s,p)}{\partial z} =$$

$$\frac{2D_e}{\delta}\left\{-\bar{C}_f(z,s,p)\sqrt{\frac{p}{D_a}} - \frac{\sqrt{s}-\sqrt{p}}{\sqrt{D_a}(p-s)}e^{-\frac{x}{u}s}\, e^{-\beta\sqrt{s}}\right\} \tag{3.43}$$

Eq. **3.43** is also a linear nonhomogeneous differential differential equation representing the flow in the fracture. The solution is given **by**

$$\bar{C}_f = \frac{1}{s}\left[1 + \frac{2\alpha}{\sqrt{p}+\sqrt{s}}\right]\left[s + p + 2\alpha(\sqrt{p}+\sqrt{s})\right]^{-1}$$

$$\left\{e^{-2\alpha\frac{(L-z)\sqrt{s}}{u}}\, e^{-\frac{(L-z)s}{u}} - e^{-\frac{L}{u}s}\, e^{-\frac{z}{u}p}\, e^{-\frac{2\alpha}{u}(\sqrt{p}z + \sqrt{s}L)}\right\} \tag{3.44}$$

where

$$\alpha = \frac{\sqrt{D_e \phi}}{\delta} \tag{3.45}$$

Since the measurements are made at the well which corresponds to $z = L$, $\bar{C}_f$ takes the form,

$$\bar{C}_f = \frac{1}{s}\left[1 + \frac{2\alpha}{\sqrt{p} + \sqrt{s}}\right]\left[\frac{1}{s + p + 2\alpha(\sqrt{p} + \sqrt{s})}\right]\left\{1 - e^{-\frac{L}{u}p}\ e^{\frac{-L}{u}s}\ e^{-2\alpha\frac{L}{u}(\sqrt{p} + \sqrt{s})}\right\} \qquad (3.46)$$

The terms $e^{-\frac{L}{u}p}$ and $e^{-\frac{L}{u}s}$ in Eq. 2.38 will cause Heaviside step function effects, $H(t_p - \frac{L}{u})$, and $H(t_f - \frac{L}{u})$ respectively,

where

$$H(x) = \begin{cases} 1 & x > 0 \\ 0 & x < 0 \end{cases} \qquad (3.47)$$

These effects are investigated as follows. The solution is in the Laplace space and is two transformations away from the real space. In this space the above solution can be exp ssed as following

$$\bar{C}_f = F(s,p,\alpha) - G(s,p,\alpha)\ e^{-\frac{L}{u}s}\ e^{-\frac{L}{u}p} \qquad (3.48)$$

In the Laplace space which is one transformation away from the real space the solution must be

$$\bar{C}_f = F(s,\tau,\alpha) - G(s,\tau - \frac{L}{U}, a)\ e^{-\frac{L}{u}s} \qquad \text{for} \quad \tau > \frac{L}{U} \qquad (3.49)$$

and

$$\bar{C}_f = F(s,\tau,\alpha) - 0 \qquad \text{for} \quad \tau < \frac{L}{u} \qquad (3.50)$$

In the real space the form of the solution has to be

$$\bar{\bar{C}}_f = F(t_j,\tau,\alpha) - G(t_j - \frac{L}{U},\tau - \frac{L}{U},\alpha) \qquad \text{for} \quad \tau > \frac{L}{U} \quad \text{and} \quad t_j > \frac{L}{U} \qquad (3.51)$$

and

$$\tilde{C}_f = F(t_j,\tau,\alpha) \qquad \text{for} \quad t_j < \frac{L}{u} \tag{3.52}$$

Since $t_j = \frac{L}{u}$ the second term will always be zero, therefore the solution becomes

$$C_f = F(t_j,t_p,\alpha)$$

or in the Laplace space,

$$\tilde{C}_f = F(s,p,\alpha)$$

and in complete form

$$\tilde{C}_f = \frac{1}{s}\left[1 + \frac{2\alpha}{\sqrt{p} + \sqrt{s}}\right]\left[\frac{1}{s + p + 2\alpha(\sqrt{p} + \sqrt{s})}\right] \tag{3.53}$$

3.22 Spike Injection Case

In tracer tests, injection of a finite size tracer slug is more common practice than the continuous tracer fluid injection. The solution for a slug injection can be obtained by superposing the continuous injection solution. In the matrix diffusion model for the continuous injection case the concentration profile in the fracture is given by Eq. 3.30

Defining

$$F = erfc\left[\frac{\alpha x}{u\sqrt{t - \frac{x}{u}}}\right] \tag{3.54}$$

and

$$C_f = C_o F$$

the slug injection solution can be written as

$$C_{fs} = C_o\left[F(t + \Delta t) - F(\Delta t)\right]$$

Since C_o in terms of the total tracer mass M, slug volume rate Q, and duration of slug injection At, is

$$C_o = \frac{M}{Q\Delta t} \tag{3.56}$$

Eq. 3.55 becomes

$$C = \frac{M}{Q\Delta t}\left[F(t + At) - F(t)\right] \tag{3.57}$$

Taking the limit, with respect to time, to obtain a spike solution,

$$C_f = \frac{M}{Q} \lim_{At \to 0} \frac{F(t + At) - F(t)}{At} \tag{3.58}$$

$$C_f = \frac{M}{Q}\frac{\partial F}{\partial t} \tag{3.59}$$

from **Eq. 3.54**

$$\frac{\partial F}{\partial t} = \frac{\alpha x}{u\sqrt{\pi(t_j - \frac{x}{u})^3}}\, e^{-\frac{a\ 4}{u^2(t_j - \frac{x}{u})}} \tag{3.60}$$

Thus the concentration profile of spike injection in the fracture at the end of the jection period (time t_j) , is

$$C_f = \frac{M}{Q}\frac{\alpha x}{u\sqrt{\pi(t_j - \frac{x}{u})^3}}\, e^{-\frac{\alpha^2 x^2}{u^2(t_j - \frac{x}{u})}} \tag{3.61}$$

Similarly the profile in the matrix can be found as

$$C_f = \frac{M}{Q}\left[\frac{2\alpha x}{u} + \sqrt{\frac{\phi}{D_e}}\, y\right]\frac{1}{2\sqrt{\pi(t_j - \frac{x}{u})^3}}\, e^{-\frac{\left[\frac{2\alpha x}{u} + \sqrt{\frac{\phi}{D_e}}\, y\right]^2}{4(t_j - \frac{x}{u})}} \tag{3.62}$$

A schematic of the profile is given in Fig. 3.6

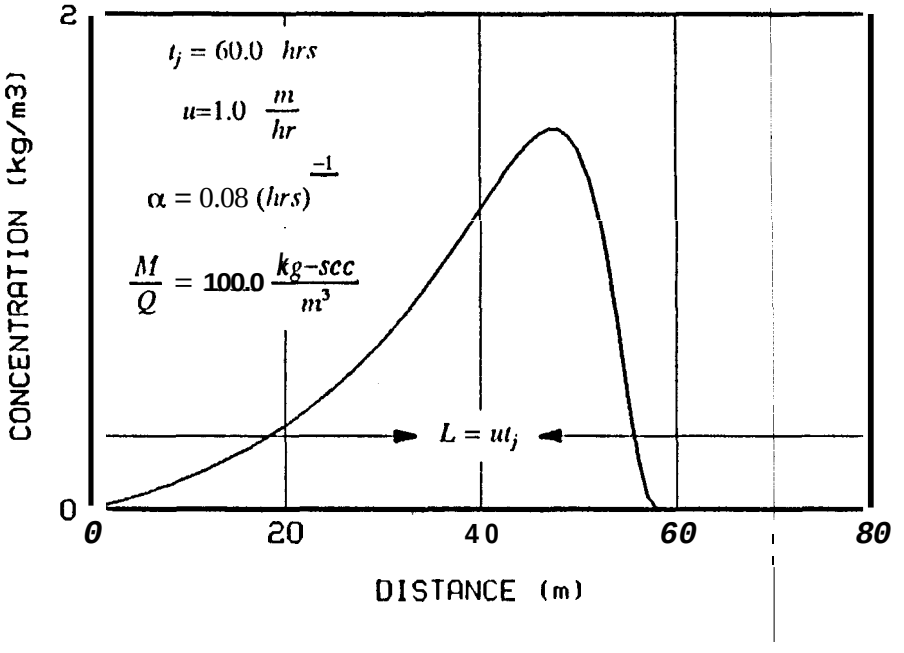

Fig. 3.6 Dispersion of a Slug Caused by Matrix Diffusion.

For the backflow period, the governing equations of the transport are the same as the equations for the continuous injection case. The boundary conditions are also the same, but the initial conditions are different. The solution for this case will also be presented in Laplace space, due to the complexity induced by the initial conditions.

The initial conditions in the Laplace space are

$$\bar{C}_f = \frac{M}{Q} e^{-\frac{xs}{u}} e^{-\left[\frac{2\alpha x}{u}\right]\sqrt{s}} \tag{3.63}$$

$$\bar{C}_p = \frac{M}{Q} e^{\frac{x}{u}} e^{-\left[\frac{2\alpha x}{u} + \sqrt{\frac{\phi}{D_e}}y\right]\sqrt{s}} \tag{3.64}$$

Since the governing equations and boundary conditions are the same, and the only difference between the initial condition Equations **3.38** and **3.63** and **3.39** and **3.64** is that $\frac{1}{s}$ term in the

former equations is replaced by $\frac{M}{Q}$ in the later ones, the solution can be written immediately from the continuous injection case.

$$\bar{C}_f = \frac{M}{Q}\left[1 + \frac{2\alpha}{\sqrt{p} + \sqrt{s}}\right]\left[\frac{1}{s + p + 2\alpha(\sqrt{p} + \sqrt{s})}\right] \tag{3.65}$$

4: ANALYSIS TECHNIQUE

The goal of the tracer tests analysis is to determine the parameters defining the flow and reservoir characteristics. In a tracer test, a fluid of constant concentration is injected into the reservoir at one well for a period of time and produced back from other wells or the same well. Then the return profiles are analyzed both qualitatively and quantitatively. This is an inverse type problem in which the input (injection) and output (return profiles) are used in interpreting the system (reservoir), whereas in a forward type problem the input and the systems characteristics are utilized to predict the output.

The quantitative analysis of an inverse problem is done by using an optimization technique to fit the model to data. In this work a nonlinear least squares curve fitting method was employed to estimate the parameters. The curve fitting was done by using a computer program **VARPRO,** (from the Stanford Center for Information Technology) which computes the optimal values for both linear and nonlinear parameters of a given function.

The method of optimization in **VARPRO** is based on a paper by Golub and Pereya. They showed that the fit of a nonlinear model of the form

$$C(E,\alpha_j,t) = \sum_{j=1}^{M} E_j\, \phi_j(\alpha_i;t) + \phi_{M+1}(\alpha_i;t) \qquad i = 1,2,3,\ldots\ldots, \tag{4.1}$$

where

C : the model to be fit

E : linear parameters

α : vector of nonlinear parameters

t : independent variable

M : number of linear parameters

ϕ : nonlinear functions

can be done by a nonlinear least squares method by optimizing the linear and nonlinear param-

eters separately.

The objective function, $R(E_j,\alpha_j)$

$$R(E_j,\alpha_j) = \sum_{i=1}^{N}\left\{C_i - \bar{C}(E_j,\alpha_j,t)\right\}^2 \qquad (4.2)$$

where

C_i : observed concentrations

$\bar{C}$: calculated concentrations

N : number of observations

is first minimized by using the initial estimates of the non-linear parameters. Then, the linear least squares procedure is applied to the residual R to obtain the values of the linear parameters. The next step is the modification of the residual by substituting the values of linear parameters. After the modification, the residual is minimized with respect to the nonlinear parameters. When the optimal values of the nonlinear parameters are computed, the linear parameters are recovered immediately. The details and the proof of the technique are discussed by *Fossum* (1982).

Since the routine uses a Taylor expansion, the derivatives of the objective function with respect to the nonlinear parameters have to be evaluated.

In the analysis the following input data are required :

1) N observed concentrations (C_i)
2) time values, t, corresponding to each observation
3) initial guesses of the nonlinear parameters

All these input data are called by the main program, which also calls for **VARPRO** and print the final results. The subroutine **ADA** called by **VARPRO,** calculates the solution with respect to the nonlinear parameters.

The solution for the continuous injection case of convection-dispersion model in the form of Eq. 4.1 is,

$$C(\alpha,t) = C_o F(t,\alpha) = C_o \frac{1}{2} erfc\left[\frac{\alpha(t_j - t_p)}{2\sqrt{t_j + t_p}}\right] \qquad (4.3)$$

where

C (a , t) : the concentration at a time t,

C_o : the concentration at inlet during the injection period

F : the nonlinear function

a : the nonlinear parameter

If we normalize the concentration dividing by C_o, we obtain

$$C_D(\alpha,t) = E\ F(t,\alpha) \tag{4.4}$$

where E is a normalization factor that normalizes the concentration to 1. The program which performs the the nonlinear least squares fitting is listed in appendix E.

Similarly the solution for the continuous injection case of the matrix diffusion model is given by

$$C_f(\alpha,t_j,t_p) = C_o F(\alpha,s,p) \tag{4.}$$

where

C_f : concentration at time t

C_o : concentration at the inlet during the injection period

F : solution in (z,s,p) space (nonlinear function)

Since the solution is available only in (z,s,p)-space the calculation of the solution and the derivatives in real space must be done numerically. Therefore, ADA needs to perform a dc ble numerical inversion

Here the procedure of the numerical evaluation technique of the solutions and derivativ will be presented by utilizing the continuos injection solution. The solution obtained at $z = L$, i.e at the wellbore was

$$\tilde{C}_f = \frac{1}{s}\left[1 + \frac{2\alpha}{\sqrt{p} + \sqrt{s}}\right]\left[\frac{1}{s + p + 2\alpha(\sqrt{p} + \sqrt{s})}\right] \qquad \text{for} \quad t_p < t_j \tag{4.6}$$

where the parameters, s, and p are the corresponding Laplace parameters of the real variables

$t_j = \frac{L}{u}$, t_p , respectively. Eq. **4.6** is analytic only in p-space. Since the p-space is two Laplace transformations away from the real space, **ADA** utilizes **three** function subprograms to perform a double numerical inversion process by using Stehfest algorithm(1970).

The main program CURFIT reads the values of the nonlinear parameters, the time steps at which the solution is to be evaluated, number of terms, **N,** that are going to be used in Stehfest algorithm and calls function **COEFF** to provide the vector v of **N** elements. Then it transfers all these parameters to subroutine **ADA,** where the solution is evaluated and **ADA** uses the Stehfest algorithm for the inversion of the solution from (z,s,t_p) space to real space. To perform the inversion, **ADA** needs the evaluation of the solution in (z,s,t_p) space and it calls the function **CDS.** The direct evaluation of the solution in (z, s, t_p) space can not be done because the solution is analytic only in (z,s,p) space. Therefore **CDS** performs another humerical inversion from (z,s,p)space to (z,s,t_p) space again by using the Stehfest algorithm. During this inversion process, function **CDS** calls the function **CDSP** for the evaluation of the solution in (z,s, p) space. The same procedure is applied for the evaluation of the derivative\$ except **DCDS** and **DCDSP** are used for the evaluations in (z,s,t_p) and (z,s,p) spaces respectively.

5: APPLICATIONS

The quantitative interpretation of the tracer return profiles can be accomplished through the application of the mathematical models to field data. So far, three different mathematical models based on different principles of dispersion in fractured media have been developed and employed in the analysis of interwell tracer tests, by other researchers. In the previous sections, two of these models have been discussed and extended for the analysis of the return profiles from the single well injection-backflow tracer tests.

Now, the results from the application of the models to field data will be presented. Both models were curve fitted to four sets of data obtained from two wells in two different geothermal fields. The curve fitting was done by using a nonlinear optimization program. Each model has only one nonlinear parameter to be determined through curve fitting.

The first two sets of the data were from a well in Raft River geothermal field. One of the sets was a 4-hour injection test and the other was a 48.5-hour injection test. The other two sets of data were from a well in East Mesa geothermal field. The first one of these sets was a 7.22-hour injection test and the injection period for the second one is 14.22 hours. From the analysis of these sets we were not only able to compare the ability of the mddels to represent the flow in the reservoir, but also analyze the effect of the injection period on the return profiles.

The the results of the curve fittings are shown in figures from Fig. 5.1 to Fig. 5.8. The first observation that we made is the matrix diffusion model gives better fit$ to all available data than the convection-dispersion model does. As far as the convection-dispersionmodel ikself is concerned it gives far better results on the small injection period tests. While the duration of injection increases fits get worse, for the convection-dispersion model.

The mamx diffusion model, on the other hand, fits all sets of the data equally well and the fits are excellent However, there is one important point has to be paid attention. The non-linear parameter of the matrix diffusion model is given by,

$$\alpha = \frac{\sqrt{D_e \phi}}{\delta} \tag{5.1}$$

In section 3.2 it was stated that D_e is a function of temperature, porosity, molecular diffusivity and the geometry of the rock. It was also assumed that the porosity and the fracture aperture is constant along the path traveled by the tracer fluid. Therefore, the values of the nonlinear parameters obtained from the analysis of the data sets of the same well have to be the same. The reason for the differing numerical values can be found in the effects of the Injection periods. Since the assumption of constant fracture aperture and uniform porosity is not absolutely true, what we obtain is an average value of those physical properties over the distance traveled by the tracer fluid. Therefore, the longer the injection period the longer the distance traveled by the fluids and, of course, the closer the the results to the true average values.

The poor fits obtained from the application of the convection-dispersion model can be explained as flow. If the injection time is short, then the amount of the tracer diffusing into the fracture will not be high, so the length of diffusion. Hence, the contribution to the dispersion within the fracture will come from the Taylor Dispersion discussed earlier in section 3.1. As the injection period increases, the effect of the interaction between the adjacent matrix and the fluid in the fracture becomes the dominant mechanism of dispersion. For this reason, convection-dispersionmodel fails to give a good fit to the data obtained from the long Injection period tests.

The last point to be considered here is the non-unit normalized concentration value even at, $t_p = 0$, for the fit of convection-dispersion model to the data of well 2C which is shown in Fig. 5.4. In order to explain this we need to go check the injection time constraint explained in section 3.1.1. The length of the transition zone was,

$$L_f = 3.62\sqrt{\eta t} \tag{5.2}$$

It was also stated that as t increases L_f proportionally to $t^{\frac{1}{2}}$ whereas the distance traveled by the particles of fluid are proportional to t. Eventually L_f will become small cdmpared with L. Now let's look at the condition for the injection time to be satisfied so that the infinite medium solution can be applied. From the point of view of numerical calculations the argument of the error function must be greater than or equal to 2, for the value of the function to be 1. Therefore, to be able to get a unit C_D at the injection point, the following has to be satisfied. At the end of the injection period, the argument was

$$\frac{x - ut_j}{2\sqrt{\eta t_j}}$$

and at $x = 0$, we want the following inequality to be satisfied

$$\frac{L}{2\sqrt{\eta t_j}} \geq 2 \tag{5.3}$$

since it was defined that $a = \frac{u}{\sqrt{\eta}}$ and $L = ut_j$. We obtain

$$\alpha\sqrt{t_j} \geq 4 \tag{5.4}$$

If we look at the values given in Fig. 5.4 we see that

$$\alpha\sqrt{t_j} = 1.33 < 4 \tag{5.5}$$

Now there is two possible explanations can be given for this result:

1) The injection time is not enough for the theory to applicable

2) The recovered value of the nonlinear parameter is not correct. In other words the model itself is not applicable.

Of course the second explanation is the logical one because of the inability of the model to represent the long injection period tests as explained above.

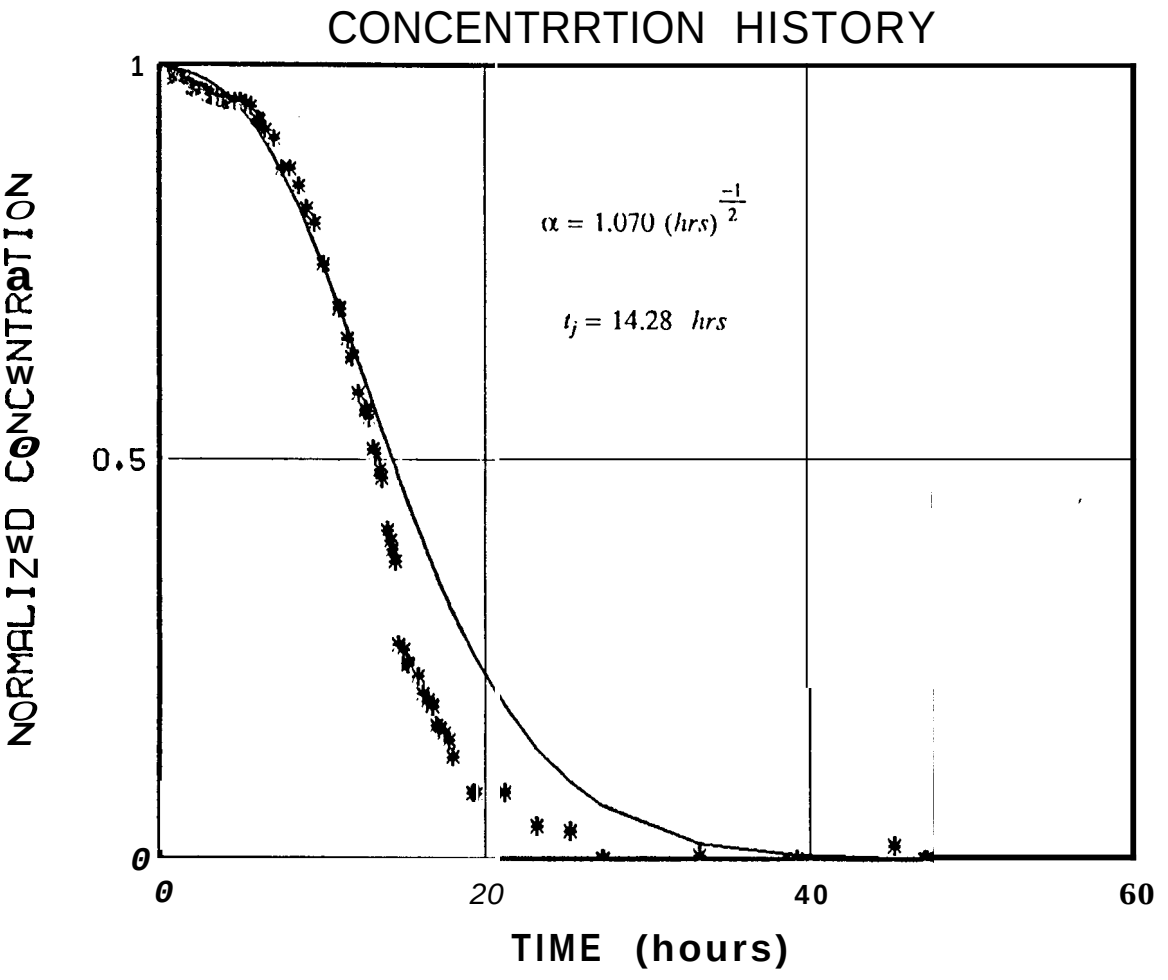

Fig. 5.2 The Result *of* Curve Fitting the Convection-Dispersion Model to the Data From well #19 test-6

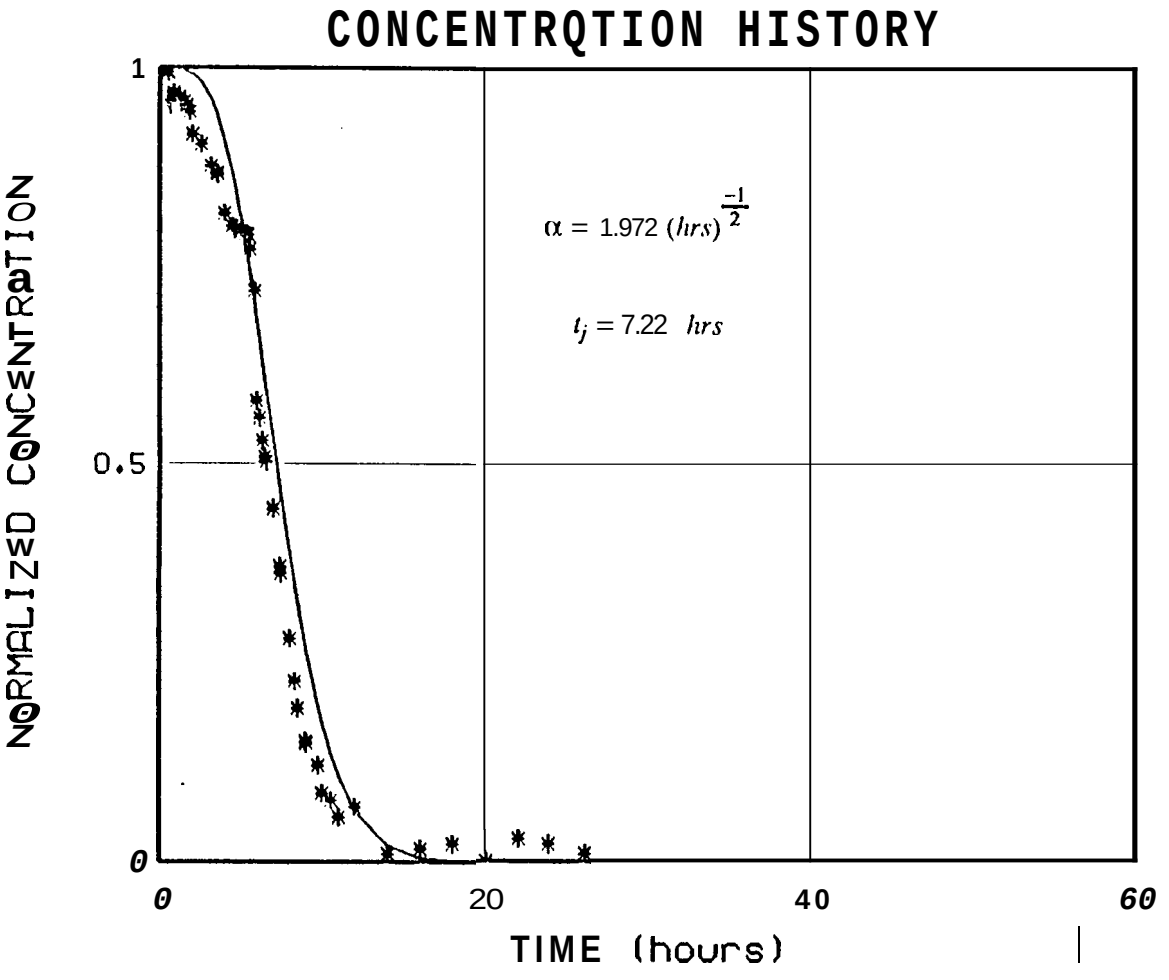

Fig. 5.1 The Result *of* Curve Fitting the Convection-Dispersion Model to the Data From well #19 test-4

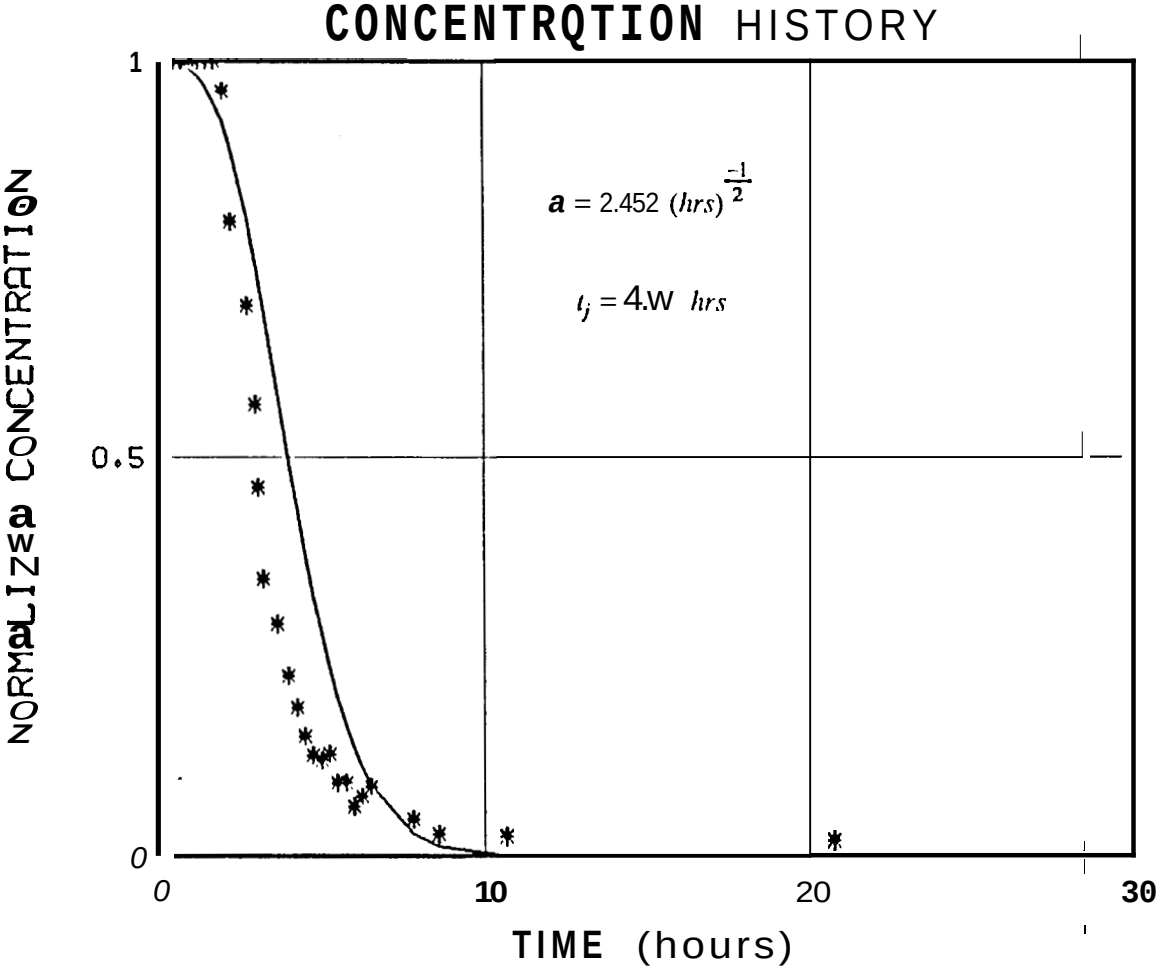

Fig. 6.3 The Result of Curve Fitting the Convection-Dispersion Model to the Data From well #2 test-a

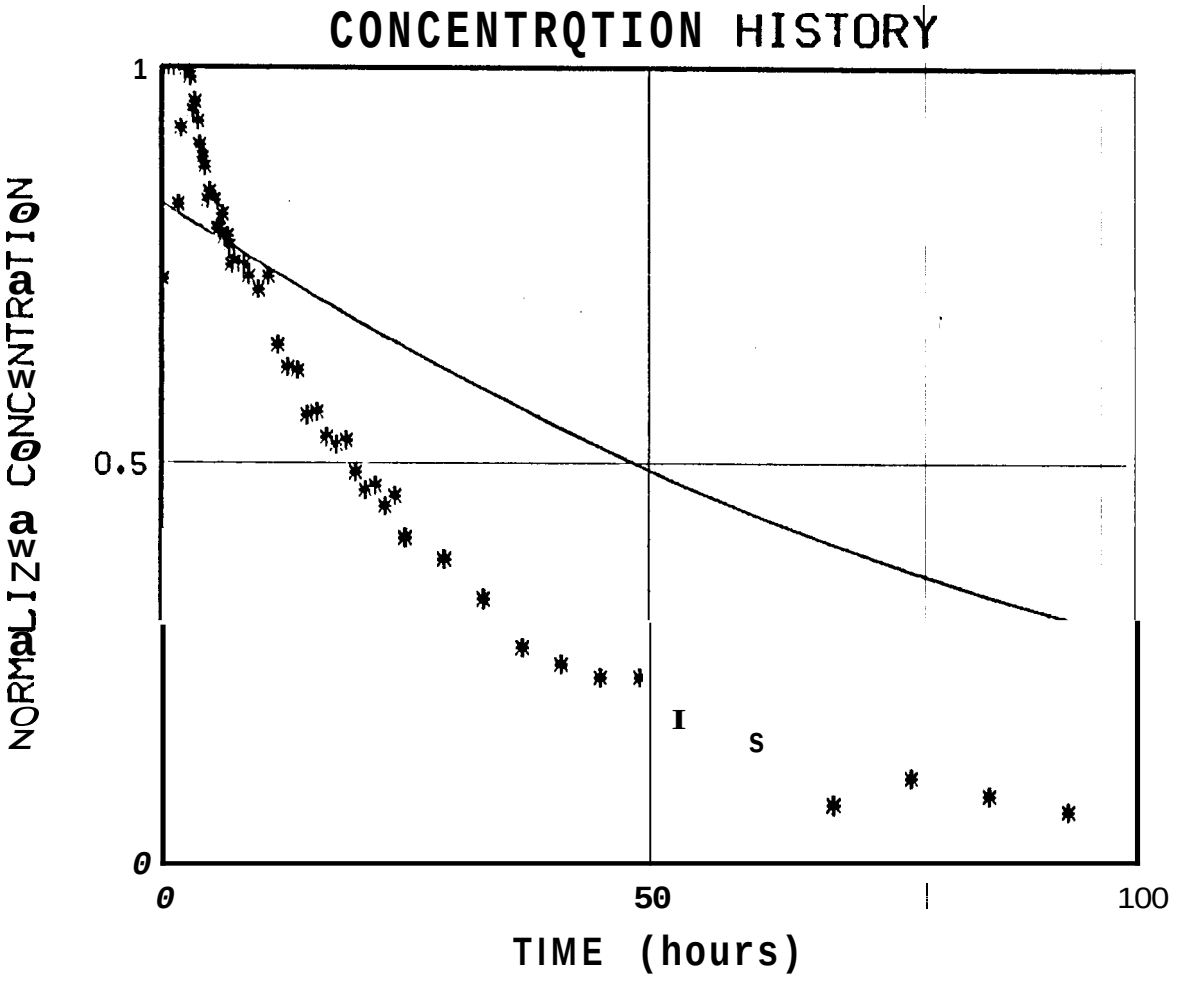

Fig. 5.4 The Result of Curve Fitting the Convection-Dispersion Model to the Data From well #2 test-c

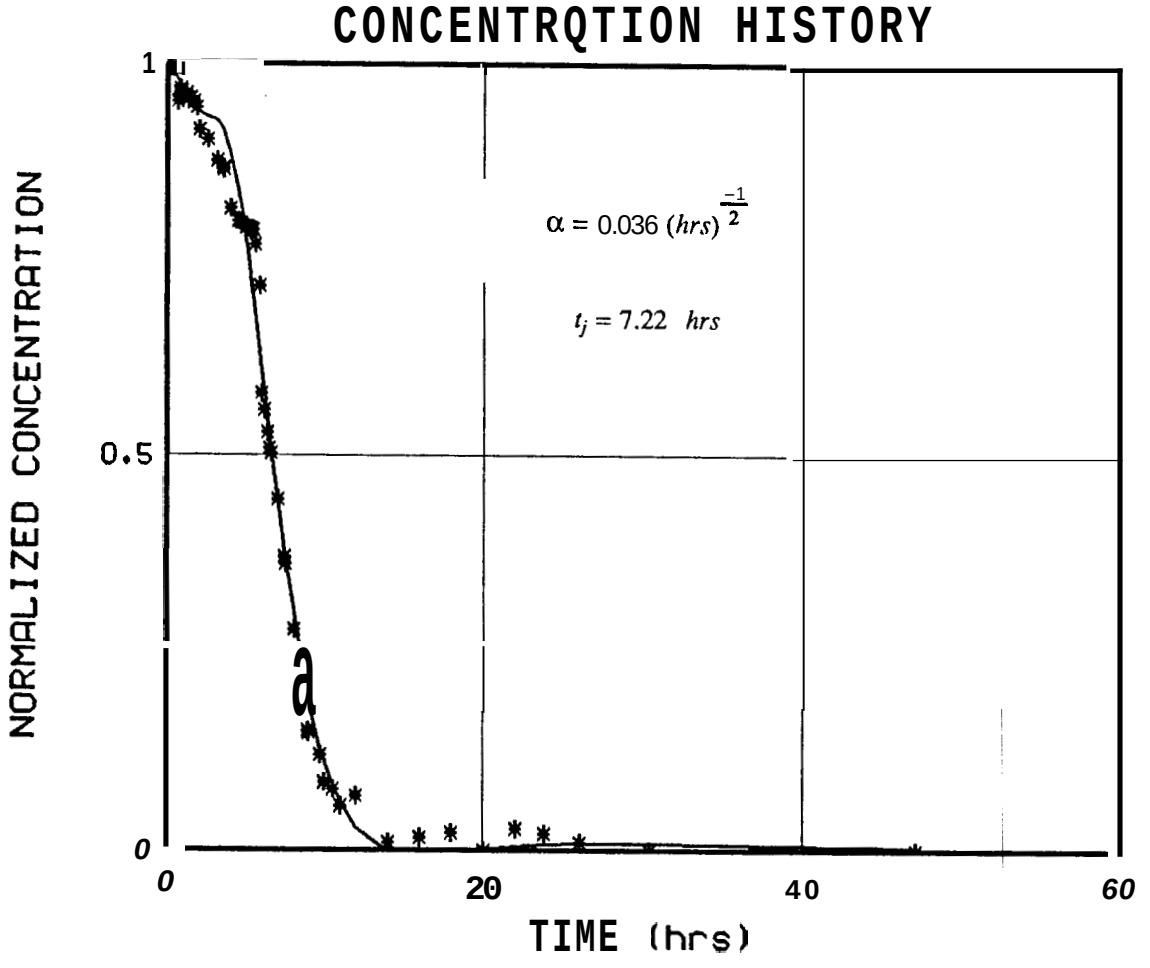

Fig. *5.5* The Result of Curve Fitting the Matrix Diffusion Model to the Data From well #19 test-4

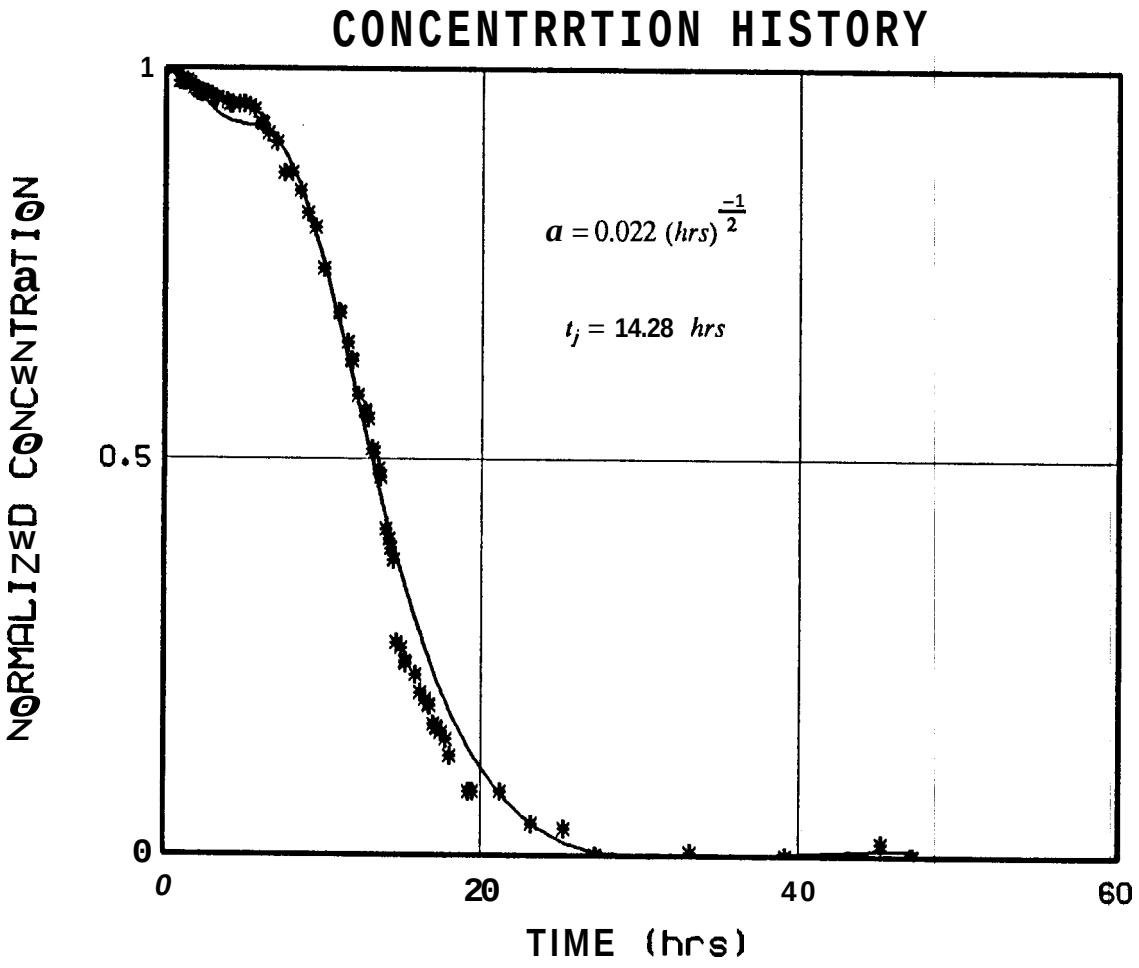

Fig. 5.8 The Result of Curve Fitting the Matrix Diffusion Model to the Data From well #19 test-6

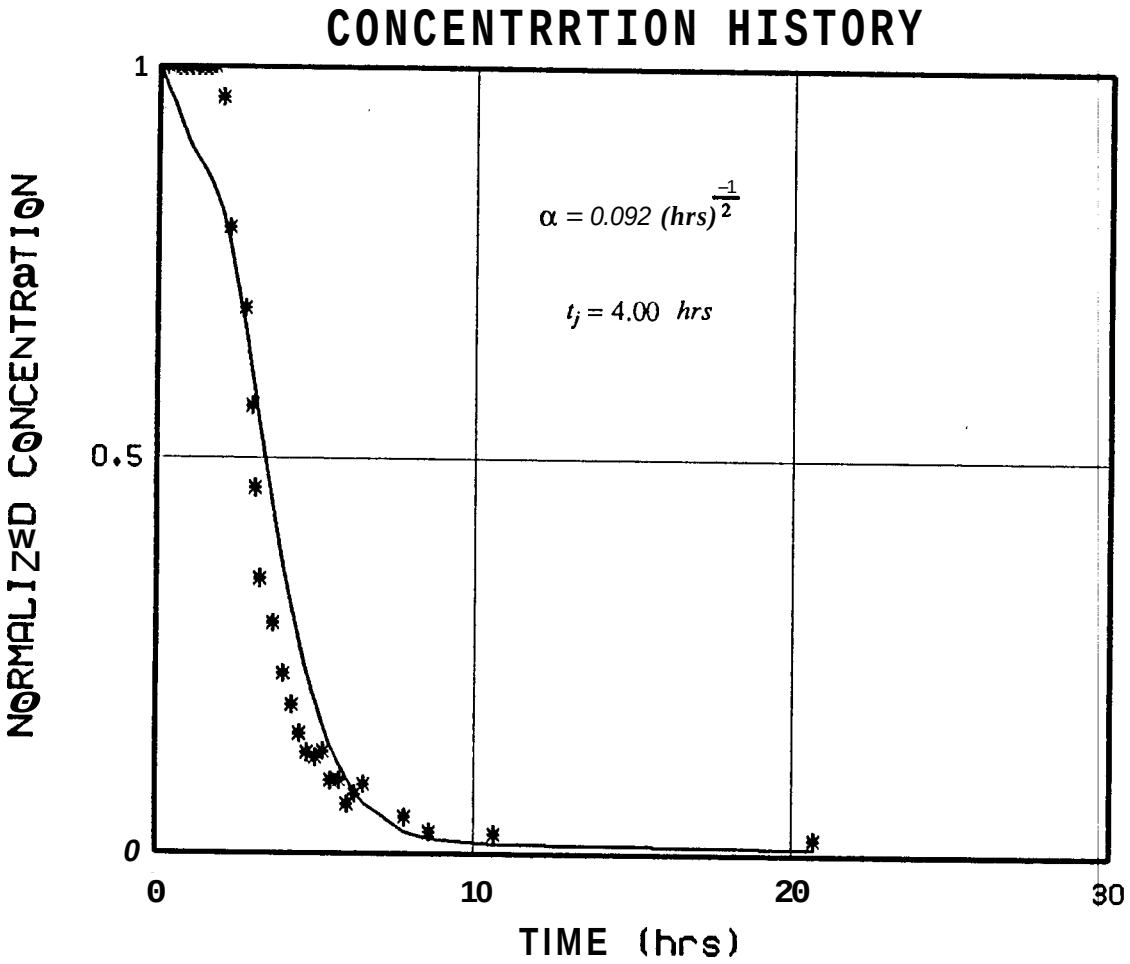

Fig. 5.7 The Result of Curve Fitting the Matrix Diffusion Model to the Data From well #2 test-a

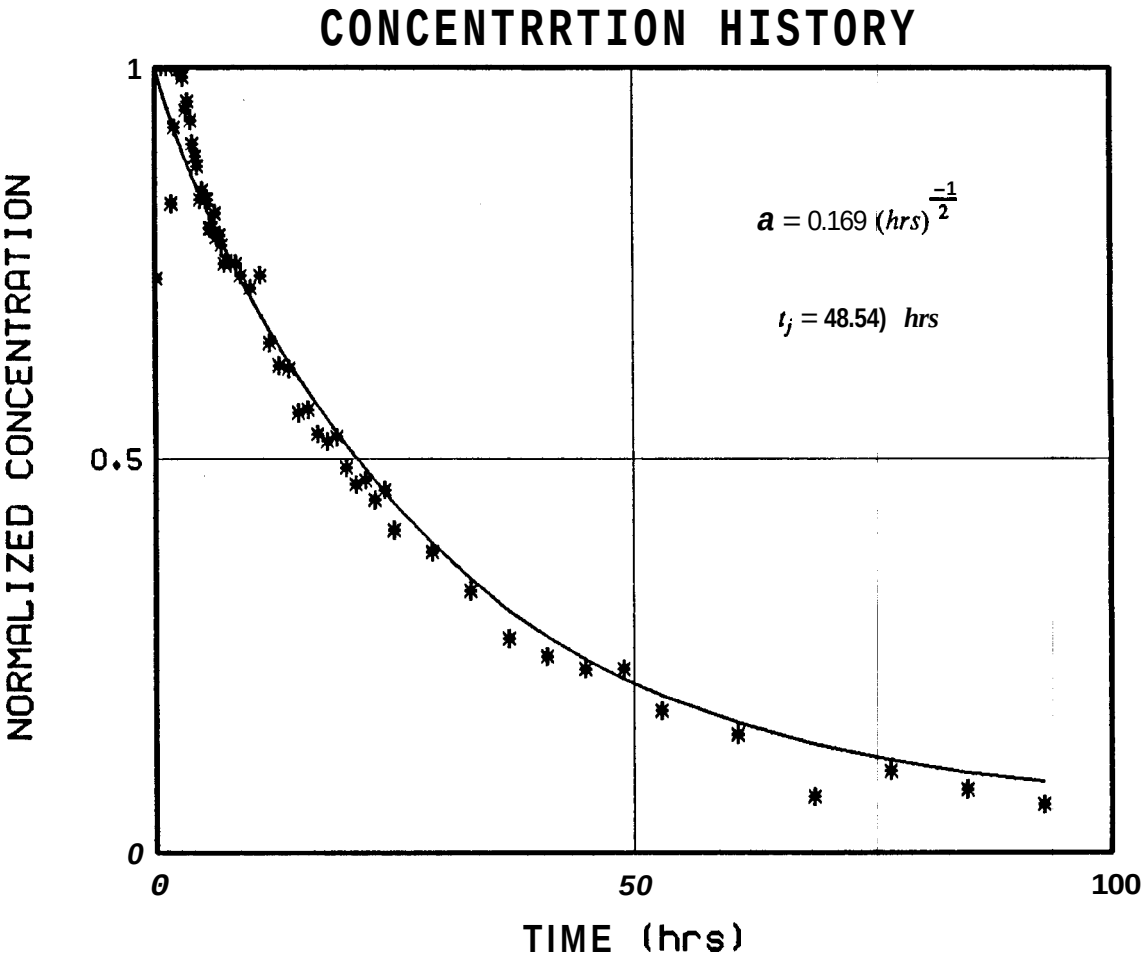

Fig. 6.8 The Result of Curve Fitting the Matrix Diffusion Model to the Data From well #2 test-c

6: CONCLUSIONS

This study has shown that the injection-backflow tracer tests can be used in determining the dispersion characteristics of the area within the radius of influence of the test well. Two mathematical models describing the tracer transport in fractured medium have been extended to the quantitative analysis of the return profiles of injection-backflow tracer tests. Then the models were used to match six sets of field data. From these fits it was seen that most of the profiles can be successfully matched by the matrix diffusion model, whereas only short term injection tests could be fitted by the convection-dispersionmodel. One suspects that the reason for this that in a short injection backflow test, the time might not be sufficient for the tracer to diffuse far enough into the porous matrix to produce the long tails in the return profile. In the case of relatively high porosity or long injection periods the return profiles are expected to be long tailed, and can be matched well by the matrix-diffusion model.

It was also observed that the parameters of models determined from fits to different data sets obtained from the same well gave different results. The differences between the two values of the same parameter were small if the injection periods were not large. In other words, the larger the difference between the injection periods the higher the difference between the determined values of the same parameter. Therefore, the injection periods should made as long as possible to obtain better average values for the governing parameters of the transport models.

7: NOMENCLATURE

CONVECTION-DISPERSION MODEL

δ : average velocity

D : molecular diffusivity

η : dispersivity coefficient

C : concentration (mass of the tracer per unit volume of the traced fluid)

$C_D = \frac{C}{C_o}$: normalized concentration

x : distance along the **flow** direction

t_j : total injection time

t_p : time variable of production period

t_i : slug injection time

$z = x - ut$: moving space coordinate

$\alpha = \frac{u}{\sqrt{\eta}}$: nonlinear parameter of the solution equation

MATRIX DIFFUSION MODEL

C_p : concentration in matrix adjacent to fracture

C_f : concentration in fracture

C_o : initial concentration of the traced fluid

D_a : apparent diffusion coefficient

D_e : effective diffusion coefficient

$K_d \rho_b$: volumetric sorption equilibrium constants

ϕ : porosity of adjacent matrix

ρ_s : solid rock density

k : adsorption distribution coefficient

x : distance along the flow direction during injection period

y : distance normal to the flow direction

z : distance along the flow direction during backflow period

$L = ut_j$: distance of the front from injection point at the end of the injection period

M : mass of tracer material

A : area open to flow

Q : volumetric injection rate of traced fluid

t_j : total injection time

τ : time variable of production period

p : Laplace parameter corresponding to production time

s : Laplace parameter corresponding to time t_j

$a = \sqrt{\frac{D_e \phi}{\delta}}$: nonlinear parameter of the solution equation

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APPENDIXES

APPENDIX A: DERIVATION OF THE CONTINUOUS INJECTION CASE SOLUTION TO MATRIX-DIFFUSION MODEL

The system of governing differential equations are,

$$\frac{\partial C_f}{\partial t} - \frac{2D_e}{\delta}\frac{\partial C_p}{\partial y}\bigg]_{y=0} + u\frac{\partial C_f}{\partial x} = 0 \qquad \text{(A1)}$$

$$D_a\frac{\partial^2 C_p}{\partial y^2} = \frac{\partial C_p}{\partial t} \qquad \text{(A2)}$$

The boundary and initial conditions are,

$$C_f = C_p = 0 \qquad at \qquad t = o$$

$$C_f = C_0 \qquad at \qquad x = o$$

$$C_p = C_f \qquad at \qquad y = o$$

$$C_p \to 0 \qquad as \qquad y \to \infty$$

If we take $C_o = 1$ then the solutions we will obtain will be the concentrations normalized by C_o.

Taking the Laplace Transform of Eq. (A2)

$$D_a\frac{\partial^2 \bar{C}_p}{\partial y^2} = s\bar{C}_p - C_p(x,0) \qquad \text{(A3)}$$

Since $C_p(x,0) = 0$, Eq. (A3) takes the form

$$D_a\frac{\partial^2 \bar{C}_p}{\partial y^2} - s\bar{C}_p = 0 \qquad \text{(A4)}$$

The solution of the above homogeneous differential equation is given by

$$\bar{C}_p = A\, e^{-\sqrt{\frac{s}{D_a}}\, y} + Be^{\sqrt{\frac{s}{D_a}}\, y} \qquad \text{(A5)}$$

Applying the boundary conditions

$$C_p \to 0 \qquad \text{as} \qquad y \to \infty \qquad \textit{implies} \qquad B = O$$

and

$$C_p = C_f \qquad \textit{at} \qquad y = 0 \quad \textit{implies} \quad A = \bar{C}_f$$

$$\bar{C}_p = \bar{C}_f\, e^{-\sqrt{\frac{s}{D_a}}\, y} \qquad \text{(A6)}$$

$$L\left\{\frac{\partial C_p}{\partial y}\right\} = \frac{\partial \bar{C}_p}{\partial y} = \frac{\partial \bar{C}_f}{\partial y}\; e^{-\sqrt{\frac{s}{D_a}}\, y} - \bar{C}_f \sqrt{\frac{s}{D_a}}\; e^{-\sqrt{\frac{s}{D_a}}\, y} \qquad \text{(A7)}$$

where L is the Laplace operator. Since

$$\frac{\partial \bar{C}_f(x,s)}{\partial y} = 0 \qquad \text{(A8)}$$

Eq.(A7) becomes

$$\frac{\partial \bar{C}_p}{\partial y} = -\,\bar{C}_f \sqrt{\frac{s}{D_a}}\; e^{-\sqrt{\frac{s}{D_a}}\, y} \qquad \text{(A9)}$$

Taking the Laplace transform of **the Eq. (A2)**

$$s\bar{C}_f - C_f(x,0) - \frac{2D_e}{\delta}\frac{\partial \bar{C}_p}{\partial y}\bigg]_{y=0} + u\frac{\partial \bar{C}_f}{\partial x} = 0 \qquad \text{(A10)}$$

since $C_f(x,0) = 0$ **, and from Eq.(A8)**

$$\frac{\partial \bar{C}_p}{\partial y}\bigg]_{y=0} = -\sqrt{\frac{s}{D_a}}\;\bar{C}_f \qquad \text{(A11)}$$

Eq. (A9) becomes

$$u\frac{\partial \bar{C}_f}{\partial x} + \left[s + \frac{2D_e}{\delta}\sqrt{\frac{s}{D_a}}\right]\bar{C}_f = 0 \qquad \text{(12)}$$

If the tracer is assumed to be inert, the relationship between the apparent and the effective diffusion coefficients is given by,

$$D_a = \frac{D_e}{\phi}$$

then

$$\frac{2D_e}{\delta}\sqrt{\frac{s}{D_a}} = \frac{2\sqrt{D_e\phi}}{\delta}\sqrt{s}$$

Let α be

$$\alpha = \frac{\sqrt{D_e\phi}}{\delta}$$

Then the equation becomes

$$u\frac{\partial \bar{C}_f}{\partial x} + \left[s + 2\alpha\sqrt{s}\right]\bar{C}_f = 0 \qquad \text{(A13)}$$

rearranging

$$\frac{\partial \bar{C}_f}{\partial x} + \left[\frac{s}{u} + \frac{2\alpha x}{u}\sqrt{s}\right]\bar{C}_f = (\qquad \text{(A14)}$$

The solution to this linear homogeneous equation is given by,

$$\bar{C}_f = A\ e^{-\frac{x}{u}s}\ e^{-\frac{2\alpha x}{u}\sqrt{s}} \qquad \text{(A15)}$$

Apply the boundary condition

$$\bar{C}_f = 1.0 \qquad \text{at} \qquad x = 0 \qquad \text{implies} \qquad A = \frac{1}{s}$$

$$\bar{C}_f = \frac{1}{s}\ e^{-\frac{x}{u}s}\ e^{-\frac{2\alpha x}{u}\sqrt{s}} \qquad \text{(A16)}$$

Thus when it is inverted to real space

$$C_f = erfc\left[\frac{\alpha x}{u\sqrt{t - \frac{x}{u}}}\right] \qquad \text{for} \qquad t > \frac{X}{U} \qquad \text{(A17)}$$

and

$$C_f = 0 \qquad \text{for} \qquad t < \frac{x}{u}$$

since the solution to Eq. (A2) was

$$\bar{C}_p = \bar{C}_f \; e^{-\sqrt{\frac{s}{D_a}}\, y} \tag{A18}$$

Inserting the expression for $\bar{C}_f$

$$\bar{C}_p = \frac{1}{s} \; e^{-\frac{x}{u}s} \; e^{-\frac{2\alpha x}{u}\sqrt{s}} \; e^{-\sqrt{\frac{\phi}{D_e}}\, y\sqrt{s}} \tag{A19}$$

and the inversion is given as

$$C_p = erfc\left\{\left[\frac{2\alpha x}{u} + \sqrt{\frac{\phi}{D_e}}\right] \frac{1}{2\sqrt{t - \frac{x}{u}}}\right\} \qquad \text{for} \qquad t > \frac{x}{u} \tag{A20}$$

and

$$C_p = 0 \qquad \text{for} \qquad t < \frac{x}{u}$$

At the end of the injection period (time t_j), the concentration profiles are given by

$$C_f = erfc\left[\frac{\alpha x}{u\sqrt{t_j - \frac{x}{u}}}\right] \qquad \text{for} \qquad t_j > \frac{x}{u} \tag{A21}$$

and

$$C_f = 0 \qquad \text{for} \qquad t_j < \frac{x}{u}$$

$$C_p = erfc\left\{\left[\frac{2\alpha x}{u} + \sqrt{\frac{\phi}{D_e}}\right] \frac{}{\sqrt{t_j - \frac{x}{u}}}\right| \qquad \text{for} \qquad t_j > \frac{}{} \tag{A22}$$

and

$$C_p = 0 \qquad \text{for} \qquad t_j < \frac{x}{u}$$

At the end of the injection period the profile in the fracture will be as in Fig.(A1).

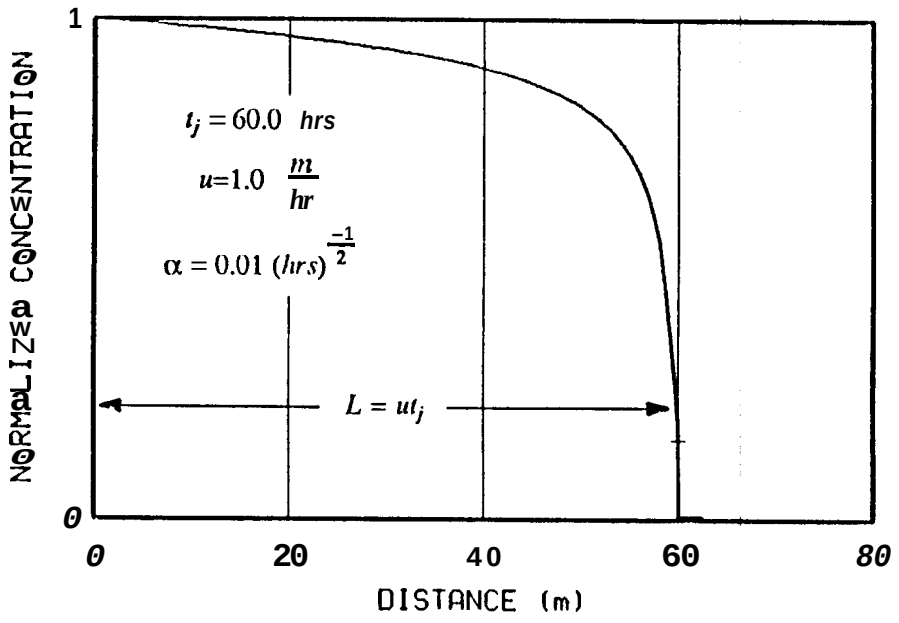

Fig. (A1) Dispersion of a Sharp Interface Caused by Matrix Diffusion.

To obtain the solutions to this period, we will work with the coordinate of space variable z and time of variable τ . We will relate x to z by $x=L-z = ut_j - z$ and take $\tau = 0$ at the beginning of the backflow period.

In the new coordinates with the assumption of equal injection and backflow rates, the governing equation of the flow in the fracture is,

$$\left[\frac{\partial C_f}{\partial \tau} - \frac{2D_a}{\delta}\frac{\partial C_p}{\partial y}\right] + u\frac{\partial C_f}{\partial z} = 0 \qquad \text{(A23)}$$

$$D_a\frac{\partial^2 C_p}{\partial y^2} = \frac{\partial C_p}{\partial \tau} \qquad \text{(A24)}$$

The boundary conditions are

$$C_f = 0 \qquad at \qquad z = 0$$
$$C_p = C_f \qquad at \qquad y = o$$

and

$$C_p \to 0 \qquad as \qquad y \to \infty$$

Here the initial conditions are the injection period solutions evaluated at time t_j. However the attempts to obtain the solutions in real space failed because of the complexity induced by the initial conditions. For this reason the Laplace transformed forms of the initial conditions were be preserved during the solutions of the equations. The initial conditions in Laplace space are given by

$$\bar{C}_f = \frac{1}{s} \; e^{-\frac{x}{u}s} \; e^{-\frac{2\alpha x}{u}\sqrt{s}} \tag{A26}$$

$$\bar{C}_p = \frac{1}{s} \; e^{-\frac{x}{u}s} \; e^{-\frac{2\alpha x}{u}\sqrt{s}} \; e^{-\sqrt{\frac{\phi}{D_e}}\, y\sqrt{s}} \tag{A27}$$

for the fracture flow and matrix-diffusion respectively. In Equations (A26) and (A27) the Laplace parameter, s, corresponds to the time of t_j .

Take the Laplace transform of the Eq. (A24) with respect to the variable τ,

$$\frac{\partial^2 \tilde{C}_f}{\partial y^2} - \frac{p}{D_a}\tilde{C}_p = \frac{-1}{s} \; \frac{e^{-\frac{x}{u}s}}{D_a} \; e^{-\frac{2\alpha x}{u}\sqrt{s}} \; e^{-\sqrt{\frac{s}{D_a}}\, y} \tag{A28}$$

Eq. (A28) is a linear nonhomogeneous differential equation and the solution is the linear combination of the homogeneous and the particular solutions. The homogeneous solution is

$$\tilde{C}_{p_h} = C_1 \, e^{\sqrt{\frac{p}{D_a}}\, y} + C_2 \; e^{-\sqrt{\frac{p}{D_a}}\, y} \tag{A29}$$

The particular solution may be found by the method of undetermined coefficients as follows. Let the particular solution be

$$\bar{C}_{p_p} = A\, e^{-\sqrt{\frac{s}{D_a}}\,y} \tag{A30}$$

From Eq. (A30)

$$\frac{d^2\bar{C}_{p_p}}{dy^2} = A\,\frac{s}{D_a}\; e^{-\sqrt{\frac{s}{D_a}}\,y} \tag{A31}$$

Substituting Equations (A30) and (A31) into Eq. (A28) we obtain

$$A\,\frac{s}{D_a}\; e^{-\sqrt{\frac{s}{D_a}}\,y} - A\,\frac{p}{D_a}\; e^{-\sqrt{\frac{s}{D_a}}\,y} = -\,\frac{e^{-\frac{x}{u}s}}{sD_a}\; e^{-\frac{2\alpha x}{u}\sqrt{s}}\; e^{-\sqrt{\frac{s}{D_a}}\,y} \tag{A32}$$

Solving for A

$$A = \frac{1}{s(p-s)}\; e^{-\frac{x}{u}s}\;\; e^{-\frac{2\alpha x}{u}\sqrt{s}} \tag{A33}$$

Inserting the value of A in Eq. (A30) the particular solution can be written as,

$$\bar{C}_{p_p} = \frac{1}{s(p-s)}\; e^{-\frac{x}{u}s}\;\; e^{-\frac{2\alpha x}{u}\sqrt{s}}\; e^{-\sqrt{\frac{s}{D_a}}\,y} \tag{A34}$$

Then the complete solution becomes,

$$\bar{C}_p = C_1\, e^{\sqrt{\frac{p}{D_a}}\,y} + C_2\; e^{-\sqrt{\frac{p}{D_a}}\,y} + \frac{1}{s(p-s)}\; e^{-\frac{x}{u}s}\;\; e^{-\frac{2\alpha x}{u}\sqrt{s}}\; e^{-\sqrt{\frac{s}{D_a}}\,y} \tag{A35}$$

Apply the boundary conditions

$$C_p \to 0 \qquad \text{as} \quad y \to \infty \quad \textit{implies} \quad C_1 = 0$$

and

$$C_p = C_f \qquad \textit{at} \qquad y = o$$

implies

$$C_2 = \bar{C}_f - \frac{1}{s\,(p-s)}\; e^{-\frac{x}{u}s}\;\; e^{-\frac{2\alpha x}{u}\sqrt{s}}$$

Let

$$\beta = e^{-\frac{x}{u}s} \quad e^{-\&E\&}$$

Then

$$\tilde{C}_p = \tilde{C}_f e^{-\sqrt{\frac{s}{D_a}}y} - \frac{\beta}{s(p-s)}\left[e^{-\sqrt{\frac{p}{D_a}}y} - e^{-\sqrt{\frac{s}{D_a}}y}\right] \tag{A36}$$

and

$$\left.\frac{\partial \tilde{C}_p}{\partial y}\right]_{y=0} = -\sqrt{\frac{p}{D_a}}\tilde{C}_f - \frac{\beta}{s(p-s)}\left[\sqrt{\frac{s}{D_a}} - \sqrt{\frac{p}{D_a}}\right] \tag{A37}$$

Now, if we take the Laplace transform of Eq. (A23) and insert Eq.(A37) we obtain,

$$p\tilde{C}_f - \bar{C}_f(z,s) - \frac{2D_e}{\delta}\left[-\tilde{C}_f\sqrt{\frac{p}{D_a}} - \frac{\sqrt{s}-\sqrt{p}}{\sqrt{D_a}(p-s)}\frac{\beta}{s}\right] + u\frac{\partial \tilde{C}_f}{\partial z} = 0 \tag{A38}$$

where $\bar{C}_f(z,s)$ is given by Eq. (A26). Rearranging Eq. (A38)

$$\frac{\partial \tilde{C}_f}{\partial z} + \left[\frac{p}{u} + \frac{2\alpha}{u}\sqrt{s}\right]\tilde{C}_f = \left[\frac{1}{su} + \frac{2\alpha}{su(\sqrt{s}+\sqrt{p})}\right] e^{-\frac{x}{u}s} \quad e^{-\frac{2\alpha x}{u}\sqrt{s}} \tag{A39}$$

Since $x = L - z$, Eq. (A39) can be rewritten as

$$\frac{\partial \tilde{C}_f}{\partial z} + \left[\frac{p}{u} + \frac{2\alpha}{u}\sqrt{s}\right]\tilde{C}_f = \omega \quad e^{\frac{z}{u}s} \quad e^{\frac{2\alpha z}{u}\sqrt{s}} \tag{A40}$$

where

$$\omega = \frac{1}{s}\left[\frac{1}{u} + \frac{2\alpha}{u(\sqrt{s}+\sqrt{p})}\right] e^{-\frac{L}{u}s} \quad e^{-\frac{2\alpha L}{u}\sqrt{s}}$$

Equation (A40) is a linear nonhomogeneous first order equation and its solution can be found by separation of variables

$$\tilde{C}_f \quad e^{\frac{z}{u}p} \quad e^{\frac{2\alpha z}{u}\sqrt{p}} = \omega \int e^{\frac{z}{u}s} \quad e^{\frac{2\alpha z}{u}\sqrt{s}} \quad e^{\frac{z}{u}p} \quad e^{\frac{2\alpha z}{u}\sqrt{p}} \, dz + A \tag{A41}$$

where A is a constant, and the solution can be rewritten as

$$\bar{C}_f = \frac{\omega}{\frac{s+p}{u} + \frac{2\alpha}{u}(\sqrt{s}+\sqrt{p})} \quad e^{\frac{z}{u}s} \; e^{\frac{2\alpha z}{u}\sqrt{s}} + A \quad e^{-\frac{z}{u}p} \; e^{-\frac{2\alpha z}{u}\sqrt{p}} \qquad \text{(A42)}$$

Applying the boundary condition, $C_f = 0$ *at* $z = 0$

$$A = -\frac{\omega}{\frac{s+p}{u} + \frac{2\alpha}{u}(\sqrt{s}+\sqrt{p})}$$

inserting the value of **A** into Eq.(A42), the backflow period solution is obtained

$$C_f = \frac{1}{s}\left[1 + \frac{2\alpha}{\sqrt{s}+\sqrt{p}}\right]\left[\frac{1}{s+p+2\alpha(\sqrt{s}+\sqrt{p})}\right]$$
$$\left\{ e^{-\frac{L}{u}s} \; e^{-\frac{2\alpha L}{u}\sqrt{s}} \; e^{\frac{z}{u}s} \; e^{\frac{2\alpha z}{u}\sqrt{s}} - e^{-\frac{L}{u}s} \; e^{-\frac{2\alpha L}{u}\sqrt{s}} \; e^{-\frac{z}{u}p} \; e^{-\frac{2\alpha z}{u}\sqrt{p}} \right\} \qquad \text{(A43)}$$

Since the concentration measurements *are* made at the well which corresponds to $z = L$

$$\bar{C}_f = \frac{1}{s}\left[1 + \frac{2\alpha}{\sqrt{s}+\sqrt{p}}\right]\left[\frac{1}{s+p+2\alpha\sqrt{s}+\sqrt{p}}\right]$$
$$\left\{1 - e^{-\frac{z}{u}(p+s)} \; e^{-\frac{2\alpha L}{u}(\sqrt{p}+\sqrt{s})}\right\} \qquad \text{(A44)}$$

In **Eq.** (A44) the terms, $e^{-\frac{L}{u}p}$ and $e^{-\frac{L}{u}s}$ will cause Heaviside step function effects, $H(t_p - \frac{L}{u})$, and $H(t_f - \frac{L}{u})$ respectively,

where

$$H(x) = \begin{cases} 1 & x > 0 \\ 0 & x < 0 \end{cases}$$

These effects **are** investigated **as** follows. The solution is in the Laplace space and it is two transformations away from the real space. In this space the above solution can be expressed in a general form **as** following.

$$\bar{C}_f = F(s,p,\alpha) - G(s,p,\alpha) \; e^{-\frac{L}{u}s} \; e^{-\frac{L}{u}p}$$

In the Laplace space which is one transformation away from the real space the solution must be

$$\bar{C}_f = F(s,\tau,\alpha) - G(s,\tau - \frac{L}{u}, a)\, e^{-\frac{L}{u}s} \qquad \text{for} \quad \tau > \frac{L}{u}$$

and

$$\bar{C}_f = F(s,\tau,\alpha) - 0 \qquad \text{for} \quad \tau < \frac{L}{u}$$

In the real space the form of the solution has to be

$$\bar{C}_f = F(t_j,\tau,\alpha) - G(t_j - \frac{L}{u}, \tau - \frac{L}{u}, a) \qquad \text{for} \quad \tau > \frac{L}{u} \qquad \text{and} \qquad t_j > \frac{L}{u}$$

and

$$\bar{C}_f = F(t_j,\tau,\alpha) \qquad \text{for} \quad t_j < \frac{L}{u}$$

Since $t_j = \frac{L}{u}$ the second term will always be zero, therefore the solution becomes

$$C_f = F(t_j,\tau,\alpha)$$

or in the Laplace space,

$$\tilde{C}_f = F(s,p,\alpha)$$

and in complete form

$$\tilde{C}_f = \frac{1}{s}\left[1 + \frac{2\alpha}{\sqrt{p} + \sqrt{s}}\right]\left[\frac{1}{s + p + 2\alpha(\sqrt{p} + \sqrt{s})}\right] \qquad \text{(A45)}$$

APPENDIX B : DERIVATIVES OF THE SOLUTIONS OF THE MATRIX DIFFUSION MODEL WITH RESPECT TO THE NONLINEAR PARAMETERS

The solution found for the continuous injection case is :

$$\tilde{C}_f = \frac{1}{s}\left[1 + \frac{2\alpha}{\sqrt{p}+\sqrt{s}}\right]\left[\frac{1}{s+p+2\alpha(\sqrt{p}+\sqrt{s})}\right] \qquad \text{(B1)}$$

The equation (B1) has only one parameter a, and the derivative with respect toia is given by

$$\frac{\partial \tilde{C}_f}{\partial \alpha} = \frac{1}{s}\left[\frac{2}{\sqrt{s}+\sqrt{p}}\,\frac{1}{s+p+2\alpha(\sqrt{p}+\sqrt{s})}\right]$$

$$-\frac{1}{s}\left[\left[1 + \frac{2\alpha}{\sqrt{p}+\sqrt{s}}\right]\frac{2(\&+\sqrt{p})}{s+p+2\alpha(\sqrt{p}+\sqrt{s})^2}\right] \qquad \text{(B2)}$$

The solution for the spike injection case is :

$$\tilde{C}_f = \frac{M}{Q}\left[1 + \frac{2\alpha}{\sqrt{p}+\sqrt{s}}\right]\left[\frac{1}{s+p+2\alpha(\sqrt{p}+\sqrt{s})}\right] \qquad \text{(B3)}$$

Equation (B3) has only one parameter a , and derivative with respect to α is given by

$$\frac{\partial \tilde{C}_f}{\partial \alpha} = \frac{M}{Q}\left[\frac{2}{\sqrt{s}+\sqrt{p}}\,\frac{1}{s+p+2\alpha(\sqrt{p}+\sqrt{s})}\right]$$

$$-\frac{M}{Q}\left[\left[1 + \frac{2\alpha}{\sqrt{p}+\sqrt{s}}\right]\frac{2(\sqrt{s}+\sqrt{p})}{s+p+2\alpha(\sqrt{p}+\sqrt{s})^2}\right] \qquad \text{(B4)}$$

APPENDIX C : DERIVATIVES OF THE SOLUTIONS OF THE CONVECTION-DISPERSION MODEL WITH RESPECT TO THE NONLINEAR PARAMETERS

The solution found for the continuous injection case is :

$$C = \frac{1}{2} + \frac{1}{2} erf\left[\frac{\alpha(t_j - t_p)}{2\sqrt{t_j + t_p}}\right] \qquad (C1)$$

The partial derivative of the erf (a c) with respect to a is given by

$$\frac{\partial erf(\alpha c)}{\partial \alpha} = \frac{2c}{\sqrt{\pi}} \; e^{-(\alpha c)^2} \qquad (C2)$$

Then the derivative of equation (C1) with respect to a can be found as

$$\frac{\partial C}{\partial \alpha} = \frac{1}{2\sqrt{\pi}} \; \frac{t_j - t_p}{\sqrt{t_j + t_p}} \; e^{\frac{-\alpha^2 (t_j - t_p)^2}{4(t_j + t_p)}} \qquad (C3)$$

The solution for the spike injection case was found as

$$C = \frac{\alpha t_i}{2\sqrt{\pi(t_j + t_p)}} \; e^{\frac{-\alpha^2 (t_j - t_p)^2}{4(t_j + t_p)}} \qquad (C4)$$

Here the nonlinear parameter is also Q and the derivative with respect to it is given by

$$C = \frac{t_i}{2\sqrt{\pi(t_j + t_p)}} \left[1 - \frac{\alpha^2(t_j - t_p)}{2(t_j + t_p)}\right] e^{\frac{-\alpha^2 (t_j - t_p)^2}{4(t_j + t_p)}} \qquad (C5)$$

APPENDIX D: Listing of Programs to Perform Nonlinear Curve Fitting of the Matrix Diffusion Model With a Sample Input and a Corresponding Output

```
C
C       LISTING OF THE CURFITTING PROGRAM FOR THE MATRIX DIFFUSION MODEL
C
C     ********************************************************************************
C     ********************************************************************************
C                 PROGRAM BEGINS
C     ********************************************************************************
C                 MAIN PROGRAM ( PROGRAM CURFIT )
C
C     ********************************************************************************
C
C                 DEFINITION OF THE PRARAMETERS
C
C                 NI : NUMBER OF TERMS THAT WILL BE USED IN STEHFEST ALGORITHM
C
C                 V  : THE VECTOR GENERATED AND USED BY THE STEHFEST ALGORITHM
C                      FOR INVERSION
C
C                 TJ : INJECTION PERIOD
C
C                 T(I): TIME STEPS AT WHICH THE CONCENTRATIONS ARE MEASURED
C                       DURING BACKFLOW PERIOD
C
C                 C : CONCENTRATIONS CALCULATED BY USING THE OPTIMUM VALUE
C                     OF THE NONLINEAR PARAMETER
C
C     ********************************************************************************
C
C                 INPUT DATA ARE STORED IN FILE "LAPLS"
C
C                 OUTPUT DATA ARE STORED IN FILE "OUTPUT"
C
C                 VALUES OF THE THE NONLINEAR PARAMETER AND OTHER STATISTICAL
C
C                 DATA ARE DISPLAYED ON THE SCREEN TOO
C
C
C
C
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION Y(100),T(100),ALF(2),BETA(2),W(100),A(100,6)
     *,C(100),INC(3,3),V(50)
      EXTERNAL ADA
      COMMON NI,V,TJ
      DATA NI/10/
      OPEN(UNIT=8,FILE='LAPLS')
      OPEN(UNIT=9,FILE='OUTFILE')
C
C
C     SET PARAMETERS FOR VARPRO
C
C
        NMAX=100
        LPP2=3
        IPRINT=1
      READ(8,*)TJ
      WRITE(6,121) TJ
  121 FORMAT(1H0,10X,'INJECTION TIME'//(F7.2))
```

```
C
C
C
      CALL COEFF(NI,V)
C     READ DATA
C
C
C     NL IS THE NUMBER OF NONLINEAR PARAMETERS
C
C
      READ(8.10 )NL
10    FORMAT(I3)
      WRITE(9,12)NL
12     FORMAT(1HØ,1ØX,'NUMBER OF NONLINEAR PARAMETERS'//(I3))
C
C
C     ESTIMATES OF THE NONLINEAR PARAMETERS
C
C
C
      READ(8,15) ALF(1)
15     FORMAT(F7.3)
      WRITE(9,2Ø)ALF(1)
20     FORMAT(1HØ,1ØX,'INITIAL ESTIMATES OF NONLIN. PARAM. '//(F8.4))
C
C
C     L IS THE NUMBER OF LINEAR PARAMETERS
C
C
C
      READ(8,22) L
22     FORMAT(I3)
      WRITE(9,25)L
25     FORMAT(1HØ,1ØX,'NUMBER OF LINEAR PARAMETERS'//(I3))
C
C
C     N IS THE NUMBER OF OBSERVATIONS
C
C
C
      READ(8,3Ø)N
30     FORMAT(I3)
      WRITE(9.35 )N
35     FORMAT(1HØ,1ØX,'NUMBER OF OBSERVATIONS'//(I3))
      DO 1 I=1,N
1     W(I)=1.Ø
C
C
C     IV IS THE NUMBER OF INDEPENDENT VERIABLES
C
C
      READ(8,4Ø)IV
40     FORMAT(I3)
      WRITE(9,45)IV
45     FORMAT(1HØ,1ØX,'NUMBER OF INDEPENDENT VARIABLES '//(I3))
C
C      READ THE TIME AND MEASURED CONCENTRATION DATA T(I) AND Y(I)
C
C
C
      READ(8,55)(T(I),Y(I),I=1,N)
55     FORMAT(2(F7.3,2X))
      WRITE(9,6Ø)(T(I),Y(I),I=1,N)
```

```
   60    FORMAT(1HØ,1ØX,'INDEPENDENT VARIABLES'//,2(F7.3,3X))
C
C
C
      CALL VARPRO(L,NL,N,NMAX,LPP2,IV,T,Y,W,ADA,A,IPRINT,ALF,BETA,
     *IERR)
C
C
C
      WRITE(9,21)
   21 FORMAT(1HØ,'CALCULATED CONCENTRATIONS',/,T5,'TIME',T15,
     *'CONCENTRATION',//)
      DO 27 I-l.N
      TD=T(I)
      CD=Ø.Ø
      AS=DLOG(2.DØ)/TJ
      DO 37 J=1,NI
      ARG=AS*J
      CD=CD+V(J)*CDS(ARG,J,TD,ALF)
   37 CONTINUE
      C(I)=CD*AS
      WRITE(9,23)T(I),C(I)
   23 FORMAT(2(F7.3,2X))
   27 CONTINUE
      STOP
      END
```

```
C
C     ************************************************************************
C     ************************************************************************
C                 PROGRAM BEGINS
C     ************************************************************************
C                 SUBROUTINE ADA
C
C     ************************************************************************
C
C     THE MATRIX A IS ARRANGED ACCORDING TO NO LINEAR PARAMETER ASSUMPTION
C
C     IF TAKE L=1 THEN HAVE TO REARRANGE IT.
C
C     ************************************************************************
C
C
C
      SUBROUTINE ADA(L,NL,N,NMAX,LPP2,IV,A,INC,T,ALF,ISEL)
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION ALF(2),A(100,6),T(100),INC(3,3),B(100,6),Y(100)
      DIMENSION V(50)
      COMMON NI,V,TJ
C
C
C     SKIP UNLESS ISEL=1
C
C
      IF(ISEL.EQ.2)GO TO 90
      IF(ISEL.EQ.3)GO TO 165
C
C     SET INCIDENCE MATRIX, INC(K,J)=1 IF ALF(K) APPEARS IN PHI(J)
C
        INC(1,1)=1.0
        WRITE(9,70) INC(1,1)
   70    FORMAT(1H0,'INCIDENCE MATRIX INC(1,1)= '//(I3))
C
C     CALCULATE MATRIX A
C
C     STORE VALUES OF THE FUNCTION IN FIRST COLUMN OF A
C
   90 DO 81 I=1,N
      TD=T(I)
      CD=0.0
      AS=DLOG(2.D0)/TJ
      DO 15 J=1,NI
      ARG=AS*J
      CD=CD+V(J)*CDS(ARG,J,TD,ALF)
   15 CONTINUE
      CD=CD*AS
      A(I,1)=CD
   81 CONTINUE
C       WRITE(9,103)(A(I,1),I=1,N)
C  103   FORMAT(1H0,'COLUMN #1 OF A(I,J) MATRIX'//(F9.5))
C
C     SKIP EVALUATION OF DERIVATIVES IF ISEL=2
C
C     STORE VALUES OF THE DERIVATIVES IN SECOND COLUMN OF A
C
      IF(ISEL.EQ.2)GO TO 200
  165 DO 170 I=1,N
      TD=T(I)
      DCD=0.0
      AS=DLOG(2.D0)/TJ
      DO 175 J=1,NI
```

```
      ARG=AS*J
      DCD=DCD+V(J)*DCDS(ARG,J,TD,ALF)
  175 CONTINUE
      DCD=DCD*AS
      A(I,2)=DCD
  170 CONTINUE
C     WRITE(9,180)(A(I,2),I=1,N)
C 180   FORMAT(1H0,'COLUMN #2 OF A(I,J) MATRIX'//(F9.5,2X))
  200 CONTINUE
      RETURN
      END
C
C
C
C     EVALUATION OF THE SOLUTION IN ( Z,S,PRODUTION TIME)-SPACE
C
      FUNCTION CDS(S,J,TD,ALF)
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION V(50),ALF(2)
      COMMON NI,V,TJ
      CDS=0.0
      AP=DLOG(2.D0)/TD
      DO 20 I=1,NI
      ARG=AP*I
      CDS=CDS+V(I)*CDSP(ARG,I,S,ALF)
   20 CONTINUE
      CDS=CDS*AP
      RETURN
      END
C
C
C
C     EVALUATION OF THE SOLUTION IN (Z,S,P)-SPACE
C
      FUNCTION CDSP(P,I,S,ALF)
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION ALF(2),V(50)
      COMMON NI,V,TJ
      F1=1.0/S*(1.0+2.0*ALF(1)/(DSQRT(S)+DSQRT(P)))
      F2=1.0/(S+P+2.0*ALF(1)*(DSQRT(S)+DSQRT(P)))
      CDSP=F1*F2
      RETURN
      END
C
C
C
C     EVALUATION OF THE DERIVATIVE OF THE SOLUTION WITH RESPECT TO
C
C     THE NONLINEAR PARAMETER IN (Z,S,PRODUCTION TIME)-SPACE .
C
      FUNCTION DCDS(S,J,TD,ALF)
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION V(50)
      COMMON NI,V,TJ
      DCDS=0.0
      AS=DLOG(2.0D0)/TD
      DO 20 I=1,NI
      ARG=AS*I
      DCDS=DCDS+V(I)*DCDSP(ARG,I,S,ALF)
   20 CONTINUE
      DCDS=DCDS*AS
      RETURN
      END
C
```

```
C
C
C       EVALUATION OF THE DERIVATIVE OF THE SOLUTION WITH RESPECT TO
C
C       THE NONINEAR SOLUTION IN (Z,S,P)-SPACE
C
        FUNCTION DCDSP(P,I,S,ALF)
        IMPLICIT REAL*8(A-H,O-Z)
        DIMENSION ALF(2),V(50)
        COMMON NI,V,TJ
        FA=DSQRT(S)+DSQRT(P)
        FB=(S+P+2.0*ALF(1)*FA)
        FC=(1.0+2.0*ALF(1)/FA)
        DCDSP=2.0/S*(1.0/(FA*FB)-FC*FA/FB**2)
        RETURN
        END
```

```
      SUBROUTINE VARPRO (L, NL, N, NMAX, LPP2, IV. T, Y, W, ADA, A,
     X IPRINT, ALF, BETA, IERR)
C
C           GIVEN A SET Of N OBSERVATIONS, CONSISTING OF VALUES Y(1),
C       Y(2), ..., Y(N) OF A DEPENDENT VARIABLE Y, WHERE Y(I)
C       CORRESPONDS TO THE IV INDEPENDENT VARIABLE(S) T(I,1), T(I,2),
C       .... T(I,IV), VARPRO ATTEMPTS TO COMPUTE A WEIGHTED LEAST
C       SQUARES FIT TO A FUNCTION ETA (THE 'MODEL') WHICH IS A LINEAR
C       COMBINATION
C                                    L
C     ETA(ALF, BETA: T) = SUM BETA * PHI (ALF; T) + PHI   (ALF; T)
C                         J-1   J      J              L+I
C
C       OF NONLINEAR FUNCTIONS PHI(J) (E.G., A SUM OF EXPONENTIALS AND/
C       OR GAUSSIANS). THAT IS, DETERMINE THE LINEAR PARAMETERS
C       BETA(J) AND THE VECTOR OF NONLINEAR PARAMETERS ALF BY MINIMIZ-
C       ING
C
C                                 2     N                          2
C          NORM(RESIDUAL)  = SUM  W  * (Y  - ETA(ALF, BETA: T  ))  .
C                            I=1  I     I                    I
C
C       THE (L+1)-ST TERM IS OPTIONAL, AND IS USED WHEN IT IS DESIRED
C       TO FIX ONE OR MORE OF THE BETA'S (RATHER THAN LET THEM BE
C       DETERMINED). VARPRO REQUIRES FIRST DERIVATIVES OF THE PHI'S.
C
C                                   NOTES:
C
C       A) THE ABOVE PROBLEM IS ALSO REFERRED TO AS 'MULTIPLE
C       NONLINEAR REGRESSION'. FOR USE IN STATISTICAL ESTIMATION,
C       VARPRO RETURNS THE RESIDUALS, THE COVARIANCE MATRIX OF THE
C       LINEAR AND NONLINEAR PARAMETERS, AND THE ESTIMATED VARIANCE OF
C       THE OBSERVATIONS.
C
C       B) AN ETA OF THE ABOVE FORM IS CALLED 'SEPARABLE'. THE
C       CASE OF A NONSEPARABLE ETA CAN BE HANDLED BY SETTING L = O
C       AND USING PHI(L+1).
C
C       C) VARPRO MAY ALSO BE USED TO SOLVE LINEAR LEAST SQUARES
C       PROBLEMS (IN THAT CASE NO ITERATIONS ARE PERFORMED). SET
C       NL = O.
C
C       D) THE MAIN ADVANTAGE OF VARPRO OVER OTHER LEAST SQUARES
C       PROGRAMS IS THAT NO INITIAL GUESSES ARE NEEDED FOR THE LINEAR
C       PARAMETERS. NOT ONLY DOES THIS MAKE IT EASIER TO USE, BUT IT
C       OFTEN LEADS TO FASTER CONVERGENCE.
C
C
C     DESCRIPTION OF PARAMETERS
C
C         L       NUMBER OF LINEAR PARAMETERS BETA (MUST BE .GE. OJ.
C         NL      NUMBER OF NONLINEAR PARAMETERS ALF (MUST BE .GE. Ø).
C         N       NUMBER OF OBSERVATIONS. N MUST BE GREATER THAN L + NL
C                 (I.E., THE NUMBER OF OBSERVATIONS MUST EXCEED THE
C                 NUMBER OF PARAMETERS).
C         IV      NUMBER OF INDEPENDENT VARIABLES T.
C         T       REAL N BY IV MATRIX OF INDEPENDENT VARIABLES. T(I, J)
C                 CONTAINS THE VALUE OF THE I-TH OBSERVATION OF THE J-TH
C                 INDEPENDENT VARIABLE.
C         Y       14-VECTOR OF OBSERVATIONS. ONE FOR EACH ROW OF T.
C         W       N-VECTOR OF NONNEGATIVE WEIGHTS. SHOULD BE SET TO 1'S
C                 IF WEIGHTS ARE NOT DESIRED. IF VARIANCES OF THE
C                 INDIVIDUAL OBSERVATIONS ARE KNOWN, W(I) SHOULD BE SET
C                 TO 1./VARIANCE(I).
```

```
C          INC      NL X (L+1) INTEGER INCIDENCE MATRIX.  INC(K, J) = 1 IF
C                   NON-LINEAR PARAMETER ALF(K) APPEARS IN THE J-TH
C                   FUNCTION PHI(J).  (THE PROGRAM SETS ALL OTHER INC(K, J)
C                   TO ZERO.)  IF PHI(L+1) IS INCLUDED IN THE MODEL,
C                   THE APPROPRIATE ELEMENTS OF THE (L+1)-ST COLUMN SHOULD
C                   BE SET TO 1'S.  INC IS NOT NEEDED WHEN L = 0 OR NL = 0.
C                   CAUTION:  THE DECLARED ROW DIMENSION OF INC (IN ADA)
C                   MUST CURRENTLY BE SET TO 12.  SEE 'RESTRICTIONS' BELOW.
C          NMAX     THE DECLARED ROW DIMENSION OF THE MATRICES A AND T.
C                   IT MUST RE AT LEAST MAX(N, 2*NL+3).
C          LPP2     L+P+2, WHERE P IS THE NUMBER OF ONES IN THE MATRIX INC.
C                   THE DECLARED COLUMN DIMENSION OF A MUST BE AT LAST
C                   LPPZ.  (IF L = 0, SET LPPZ = NL+2. IF NL = 0, SET LPP2
C                   L+2.)
C          A        REAL MATRIX OF SIZE MAX(N, 2*NL+3) BY L+P+2.  ON INPUT
C                   IT CONTAINS THE PHI(J)'S AND THEIR DERIVATIVES (SEE
C                   BELOW).  ON OUTPUT, THE FIRST L+NL ROWS AND COLUMNS OF
C                   A WILL CONTAIN At4 APPROXIMATION TO THE (WEIGHTED)
C                   COVARIANCE MATRIX AT THE SOLUTION (THE FIRST L ROWS
C                   CORRESPOND TO THE LINEAR PARAMETERS, THE LAST NL TO THE
C                   NONLINEAR ONES), COLUMN L+NL+1 WILL CONTAIN THE
C                   WEIGHTED RESIDUALS (Y - ETA), A(1, L+NL+2) WILL CONTAIN
C                   THE (EUCLIDEAN) NORM OF THE WEIGHTED RESIDUAL, AND
C                   A(2, L+NL+2) WILL CONTAIN AN ESTIMATE OF THE (WEIGHTED)
C                   VARIANCE OF THE OBSERVATIONS, NORM(RESIDUAL)**2
C                   (N - L - NL).
C          IPRINT   INPUT INTEGER CONTROLLING PRINTED OUTPUT.  IF IPRINT IS
C                   POSITIVE, THE NONLINEAR PARAMETERS, THE NORM OF THE
C                   RESIDUAL, AND THE MARQUARDT PARAMETER WILL BE OUTPUT
C                   EVERY IPRINT-TH ITERATION (AND INITIALLY, AND AT THE
C                   FINAL ITERATION).  THE LINEAR PARAMETERS WILL BE
C                   PRINTED AT THE FINAL ITERATION.  ANY ERROR MESSAGES
C                   WILL ALSO BE PRINTED.  (IPRINT = 1 IS RECOMMENDED AT
C                   FIRST.)  IF IPRINT = 0, ONLY THE FINAL QUANTITIES WILL
C                   BE PRINTED, AS WELL AS ANY ERROR MESSAGES.  IF IPRINT =
C                   -1. NO PRINTING WILL BE DONE.  THE USER IS THEN
C                   RESPONSIBLE FOR CHECKING THE PARAMETER IERR FOR ERRORS.
C          ALF      NL-VECTOR OF ESTIMATES OF NONLINEAR PARAMETERS
C                   (INPUT).  ON OUTPUT IT WILL CONTAIN OPTIMAL VALUES OF
C                   THE NONLINEAR PARAMETERS.
C          BETA     L-VECTOR OF LINEAR PARAMETERS (OUTPUT ONLY).
C          IERR     INTEGER ERROR FLAG (OUTPUT):
C                   .GT. 0 - SUCCESSFUL CONVERGENCE, IERR IS THE NUMBER OF
C                        ITERATIONS TAKEN.
C                   -1  TERMINATED FOR TOO MANY ITERATIONS.
C                   -2  TERMINATED FOR ILL-CONDITIONING (MARQUARDT
C                        PARAMETER TOO LARGE.)  ALSO SEE IERR = -8 BELOW.
C                   -4  INPUT ERROR IN PARAMETER N, L, NL. LPP2, OR NMAX.
C                   -5  INC MATRIX IMPROPERLY SPECIFIED, OR P DISAGREES
C                        WITH LPPZ.
C                   -6  A WEIGHT WAS NEGATIVE.
C                   -7  'CONSTANT' COLUMN WAS COMPUTED MORE THAN ONCE.
C                   -8  CATASTROPHIC FAILURE - A COLUMN OF THE A MATRIX HAS
C                        BECOME ZERO.  SEE 'CONVERGENCE FAILURES' BELOW.
C
C                   (IF IERR .LE. -4. THE LINEAR PARAMETERS, COVARIANCE
C                   MATRIX, ETC. ARE NOT RETURNED.)
C
C     SUBROUTINES REQUIRED
C
C          NINE SUBROUTINES, DPA. ORFAC1, ORFACZ. BACSUB. POSTPR, COV,
C        XNORM, INIT, AND VARERR ARE PROVIDED.  IN ADDITION, THE USER
C        MUST PROVIDE A SUBROUTINE (CORRESPONDING TO THE ARGUMENT ADA)
C        WHICH, GIVEN ALF, WILL EVALUATE THE FUNCTIONS PHI(J) AND THEIR
```

```
C       PARTIAL DERIVATIVES D PHI(J)/D ALF(K), AT THE SAMPLE POINTS
C       T(I).  THIS ROUTINE MUST BE DECLARED 'EXTERNAL' IN THE CALLING
C       PROGRAM.  ITS CALLING SEQUENCE IS
C
C       SUBROUTINE ADA (L+1, NL, N, NMAX, LPP2, IV, A, INC, T, ALF,
C       ISEL)
C
C          THE USER SHOULD MODIFY THE EXAMPLE SUBROUTINE 'ADA' (GIVEN
C       ELSEWHERE) FOR HIS OWN FUNCTIONS.
C
C          THE VECTOR SAMPLED FUNCTIONS PHI(J) SHOULD BE STORED IN THE
C       FIRST N ROWS AND FIRST L+I COLUMNS OF THE MATRIX A, I.E.,
C       A(I, J) SHOULD CONTAIN PHI(J, ALF; T(I,1), T(I,2), ...,
C       T(I,IV)), I = 1, ..., N: J = I, ..., L (OR L+1).  THE (L+1)-ST
C       COLUMN OF A CONTAINS PHI(L+1) IF PHI(L+1) IS IN THE MODEL,
C       OTHERWISE IT IS RESERVED FOR WORKSPACE.  THE 'CONSTANT' FUNC-
C       TIONS (THESE ARE FUNCTIONS PHI(J) WHICH DO NOT DEPEND UPON ANY
C       NONLINEAR PARAMETERS ALF, E.G., T(I)**J) (IF ANY) MUST APPEAR
C       FIRST, STARTING IN COLUMN 1.  THE COLUMN N-VECTORS OF NONZERO
C       PARTIAL DERIVATIVES D PHI(J) / D ALF(K) SHOULD BE STORED
C       SEQUENTIALLY IN THE MATRIX A IN COLUMNS L+2 THROUGH L+P+1.
C       THE ORDER IS
C
C          D PHI(1)   D PHI(2)          D PHI(L)   D PHI(L+1)   D PHI(1)
C          --------, --------* ...,     --------, ----------, --------,
C          D ALF(1)   D ALF(1)          D ALF(1)    D ALF(1)    D ALF(2)
C
C          D PHI(2)          D PHI(L+1)          D PHI(1)          D PHI(L+1)
C          --------, ...,    ----------, ....    ---------, ....   ----------,
C          D ALF(2)           D ALF(2)           D ALF(NL)         D ALF(NL)
C
C       OMITTING COLUMNS OF DERIVATIVES WHICH ARE ZERO, AND OMITTING
C       PHI(L+1) COLUMNS IF PHI(L+1) IS NOT IN THE MODEL.  NOTE THAT
C       THE LINEAR PARAMETERS BETA ARE NOT USED IN THE MATRIX A.
C       COLUMN L+P+2 IS RESERVED FOR WORKSPACE.
C
C       THE CODING OF ADA SHOULD BE ARRANGED SO THAT:
C
C       ISEL = 1  (WHICH OCCURS THE FIRST TIME ADA IS CALLED) MEANS:
C                 A.  FILL IN THE INCIDENCE MATRIX INC
C                 B.  STORE ANY CONSTANT PHI'S IN A.
C                 C.  COMPUTE NONCONSTANT PHI'S AND PARTIAL DERIVA-
C                     TIVES.
C            = 2  MEANS COMPUTE ONLY THE NONCONSTANT FUNCTIONS PHI
C            = 3  MEANS COMPUTE ONLY THE DERIVATIVES
C
C       (WHEN THE PROBLEM IS LINEAR (NL = Ø) ONLV ISEL = 1 IS USED, AND
C       DERIVATIVES ARE NOT NEEDED.)
C
C     RESTRICTIONS
C
C          THE SUBROUTINES DPA, INIT (AND ADA) CONTAIN THE LOCALLY
C       DIMENSIONED MATRIX INC, WHOSE DIMENSIONS ARE CURRENTLY SET FOR
C       MAXIMA OF L+I = 8, NL = 12.  THEY MUST BE CHANGED FOR LARGER
C       PROBLEMS.  DATA PLACED IN ARRAY A IS OVERWRITTEN ('DESTROYED').
C       DATA PLACED IN ARRAYS T, Y AND INC IS LEFT INTACT.  THE PROGRAM
C       RUNS IN WATFIV, EXCEPT WHEN L = O OR NL = O.
C
C          IT IS ASSUMED THAT THE MATRIX PHI(J, RLF: T(I)) HAS FULL
C       COLUMN RANK.  THIS MEANS THAT THE FIRST L COLUMNS OF THE MATRIX
C       A MUST BE LINEARLY INDEPENDENT.
C
C          OPTIONAL NOTE:  AS WILL BE NOTED FROM THE SAMPLE SUBPROGRAM
C       ADA, THE DERIVATIVES D PHI(J)/D ALF(K) (ISEL = 3) MUST BE
```

```
C        COMPUTED INDEPENDENTLY OF THE FUNCTIONS PHI(J) (ISEL = 2),
C        SINCE THE FUNCTION VALUES ARE OVERWRITTEN AFTER ADA IS CALLED
C        WITH ISEL = 2.  THIS IS DONE TO MINIMIZE STORAGE. AT THE POS-
C        SIBLE EXPENSE OF SOME RECOMPUTATION (SINCE THE FUNCTIONS AND
C        DERIVATIVES FREQUENTLY HAVE SOME COMMON SUBEXPRESSIONS).  TO
C        REDUCE THE AMOUNT OF COMPUTATION AT THE EXPENSE OF SOME
C        STORAGE, CREATE A MATRIX B OF DIMENSION NMAX BY L+I IN ADA, AND
C        AFTER THE COMPUTATION OF THE PHI'S (ISEL = 2), COPY THE VALUES
C        INTO B.  THESE VALUES CAN THEN BE USED TO CALCULATE THE DERIV-
C        ATIVES (ISEL = 3).  (THIS MAKES USE OF THE FACT THAT WHEN A
C        CALL TO ADA WITH ISEL = 3 FOLLOWS A CALL WITH ISEL = 2, THE
C        ALFS ARE THE SAME.)
C
C           TO CONVERT TO OTHER MACHINES, CHANGE THE OUTPUT UNIT IN THE
C        DATA STATEMENTS IN VARPRO, DPA, POSTPR, AND VARERR.  THE
C        PROGRAM HAS BEEN CHECKED FOR PORTABILITY BY THE BELL LABS PFORT
C        VERIFIER.  FOR MACHINES WITHOUT DOUBLE PRECISION HARDWARE, IT
C        MAY BE DESIRABLE TO CONVERT TO SINGLE PRECISION.  THIS CAN BE
C        DONE BY CHANGING (A) THE DECLARATIONS 'DOUBLE PRECISION' TO
C        'REAL', (B) THE PATTERN '.D' TO '.E' IN THE 'DATA' STATEMENT IN
C        VARPRO, (C) DSIGN, DSQRT AND DABS TO SIGN, SQRT AND ABS,
C        RESPECTIVELY, AND (D) DEXP TO EXP IN THE SAMPLE PROGRAMS ONLY.
C
C     NOTE ON INTERPRETATION OF COVARIANCE MATRIX
C
C           FOR USE IN STATISTICAL ESTIMATION (MULTIPLE NONLINEAR
C        REGRESSION) VARPRO RETURNS THE COVARIANCE MATRIX OF THE LINEAR
C        AND NONLINEAR PARAMETERS.  THIS MATRIX WILL BE USEFUL ONLY IF
C        THE USUAL STATISTICAL ASSUMPTIONS HOLD:  AFTER WEIGHTING, THE
C        ERRORS IN THE OBSERVATIONS ARE INDEPENDENT AND NORMALLY DISTRI-
C        BUTED, WITH MEAN ZERO AND THE SAME VARIANCE.  IF THE ERRORS DO
C        NOT HAVE MEAN ZERO (OR ARE UNKNOWN), THE PROGRAM WILL ISSUE A
C        WARNING MESSAGE (UNLESS IPRINT .LT. Ø) AND THE COVARIANCE
C        MATRIX WILL NOT BE VALID.  IN THAT CASE, THE MODEL SHOULD BE
C        ALTERED TO INCLUDE A CONSTANT TERM (SET PHI(1) = 1.).
C
C           NOTE ALSO THAT, IN ORDER FOR THE USUAL ASSUMPTIONS TO HOLD,
C        THE OBSERVATIONS MUST ALL BE OF APPROXIMATELY THE SAME
C        MAGNITUDE (IN THE ABSENCE OF INFORMATION ABOUT THE ERROR OF
C        EACH OBSERVATION), OTHERWISE THE VARIANCES WILL NOT BE THE
C        SAME.  IF THE OBSERVATIONS ARE NOT THE SAME SIZE, THIS CAN BE
C        CURED BY WEIGHTING.
C
C           IF THE USUAL ASSUMPTIONS HOLD, THE SQUARE ROOTS OF THE
C        DIAGONALS OF THE COVARIANCE MATRIX A GIVE THE STANDARD ERROR
C        S(I) OF EACH PARAMETER.  DIVIDING A(I,J) BY S(I)*S(J) YIELDS
C        THE CORRELATION MATRIX OF THE PARAMETERS.  PRINCIPAL AXES AND
C        CONFIDENCE ELLIPSOIDS CAN BE OBTAINED BY PERFORMING AN EIGEN-
C        VALUE/EIGENVECTOR ANALYSIS ON A.  ONE SHOULD CALL THE EISPACK
C        PROGRAM TRED2, FOLLOWED BY TQLP (OR USE THE EISPAC CONTROL
C        PROGRAM).
C
C     CONVERGENCE FAILURES
C
C           IF CONVERGENCE FAILURES OCCUR, FIRST CHECK FOR INCORRECT
C        CODING OF THE SUBROUTINE ADA.  CHECK ESPECIALLY THE ACTION OF
C        ISEL, AND THE COMPUTATION OF THE PARTIAL DERIVATIVES.  IF THESE
C        ARE CORRECT. TRY SEVERAL STARTING GUESSES FOR ALF.  IF ADA
C        IS CODED CORRECTLY, AND IF ERROR RETURNS IERR = -2 OR -8
C        PERSISTENTLY OCCUR, THIS IS A SIGN OF ILL-CONDITIONING, WHICH
C        MAY BE CAUSED BY SEVERAL THINGS.  ONE IS POOR SCALING OF THE
C        PARAMETERS: ANOTHER IS AN UNFORTUNATE INITIAL GUESS FOR THE
C        PARAMETERS, STILL ANOTHER IS A POOR CHOICE OF THE MODEL.
C
```

```
C     ALGORITHM
C
C        THE RESIDUAL R IS MODIFIED TO INCORPORATE, FOR ANY FIXED
C     ALF, THE OPTIMAL LINEAR PARAMETERS FOR THAT ALF.  IT IS THEN
C     POSSIBLE TO MINIMIZE ONLY ON THE NONLINEAR PARAMETERS.  AFTER
C     THE OPTIMAL VALUES OF THE NONLINEAR PARAMETERS HAVE BEEN DETER-
C     MINED.  THE LINEAR PARAMETERS CAN BE RECOVERED BY LINEAR LEAST
C     SQUARES TECHNIQUES (SEE REF. 1).
C
C        THE MINIMIZATION IS BY A MODIFICATION OF OSBORNE'S (REF. 3)
C     MODIFICATION OF THE LEVENBERG-MARQUARDT ALGORITHM.  INSTEAD OF
C     SOLVING THE NORMAL EQUATIONS WITH MATRIX
C
C              T      2
C           (J J + NU  * D),       WHERE  J = D(ETA)/D(ALF),
C
C     STABLE ORTHOGONAL (HOUSEHOLDER) REFLECTIONS ARE USED ON A
C     MODIFICATION OF THE MATRIX
C                                  (   J   )
C                                  (-------) ,
C                                  ( NU*D  )
C
C     WHERE D IS A DIAGONAL MATRIX CONSISTING OF THE LENGTHS Of THE
C     COLUMNS OF J.  THIS MARQUARDT STABILIZATION ALLOWS THE ROUTINE
C     TO RECOVER FROM SOME RANK DEFICIENCIES IN THE JACOBIAN.
C     OSBORNE'S EMPIRICAL STRATEGY FOR CHOOSING THE MARQUARDT PARAM-
C     ETER HAS PROVEN KEASONABLY SUCCESSFUL IN PRACTICE.  (GAUSS-
C     NEWTON WITH STEP CONTROL CAN BE OBTAINED BY MAKING THE CHANGE
C     INDICATED BEFORE THE INSTRUCTION LABELED 5).  A DESCRIPTION CAN
C     BE FOUND IN REF. (3), AND A FLOW CHART IN (2), P. 22.
C
C     FOR REFERENCE, SEE
C
C     1.  GENE H. GOLUB AND V. PEREYRA, 'THE DIFFERENTIATION OF
C         PSEUDO-INVERSES AND NONLINEAR LEAST SQUARES PROBLEMS WHOSE
C         VARIABLES SEPARATE,' SIAM J. NUMER. ANAL. 10, 413-432
C         (1973).
C     2.  -------, SAME TITLE, STANFORD C.S. REPORT 72-261, FEB. 1972.
C     3.  OSBORNE, MICHAEL R., 'SOME ASPECTS OF NON-LINEAR LEAST
C         SQUARES CALCULATIONS,* IN LOOTSMA, ED., 'NUMERICAL METHODS
C         FOR NON-LINEAR OPTIMIZATION,' ACADEMIC PRESS, LONDON, 1972'.
C     4.  KROGH, FRED, 'EFFICIENT IMPLEMENTATION OF A VARIABLE PRO-
C         JECTION ALGORITHM FOR NONLINEAR LEAST SQUARES PROBLEMS,'
C         COMM. ACM 17. PP. 167-169 (MARCH, 1974).
C     5.  KAUFMAN. LINDA, 'A VARIABLE PROJECTION METHOD FOR SOLVING
C         SEPARABLE NONLINEAR LEAST SQUARES PROBLEMS', B.I.T. 15,
C         49-57 (1975).
C     6.  DRAPER, N., AND SMITH, H., APPLIED REGRESSION ANALYSIS,
C         WILEY, N.Y., 1966 (FOR STATISTICAL INFORMATION ONLY).
C     7.  C. LAWSON AND R. HANSON, SOLVING LEAST SQUARES PROBLEMS,
C         PRENTICE-HALL, ENGLEWOOD CLIFFS, N. J., 1974.
C
C                    JOHN BOLSTAD
C                    COMPUTER SCIENCE DEPT.,  SERRA HOUSE
C                    STANFORD UNIVERSITY
C                    JANUARY, 1977
C
C     ..................................................................
C
      DOUBLE PRECISION A(NMAX, LPP2), BETA(L), ALF(NL), T(NMAX, IV),
     2 W(N), Y(N), ACUM, EPSI, GNSTEP, NU, PRJRES, R, RNEW, XNORM
      INTEGER B1, OUTPUT
      LOGICAL SKIP
      EXTERNAL ADA
```

```
      DATA EPSI /1.D-6/, ITMAX /40/, OUTPUT /6/
C
C           THE FOLLOWING TWO PARAMETERS ARE USED IN THE CONVERGENCE
C           TEST:  EPSI IS AN ABSOLUTE AND RELATIVE TOLERANCE FOR THE
C           NORM OF THE PROJECTION OF THE RESIDUAL ONTO THE RANGE OF THE
C           JACOBIAN OF THE VARIABLE PROJECTION FUNCTIONAL.
C           ITMAX IS THE MAXIMUM NUMBER OF FUNCTION AND DERIVATIVE
C           EVALUATIONS ALLOWED.  CAUTION:  EPSI MUST NOT BE
C           SET SMALLER THAN 10 TIMES THE UNIT ROUND-OFF OF THE MACHINE.
C
C-----------------------------------------------------------------      005
CALL LIB MONITOR FROM VARPRO, MAINTENANCE NUMBER 509, DATE 77178        006
C***PLEASE DON'T REMOVE OR CHANGE THE ABOVE CALL. IT IS YOUR ONLY       008
C***PROTECTION AGAINST YOUR USING AN OUT-OF-DATE OR INCORRECT           009
C***VERSION OF THE ROUTINE. THE LIBRARY MONITOR REMOVES THIS CALL.      01
C***SO IT ONLY OCCURS ONCE, ON THE FIRST ENTRY TO THIS ROUTINE.         011
C-----------------------------------------------------------------      012
      IERR = 1
      ITER = 0
      LP1 = L + 1
      B1 = L + 2
      LNL2 = L + NL + 2
      NLP1 = NL + 1
      SKIP = .FALSE.
      MODIT = IPRINT
      IF (IPRINT .LE. 0) MODIT = ITMAX + 2
      NU = 0.
C             IF GAUSS-NEWTON IS DESIRED REMOVE THE NEXT STATEMENT.
      NU = 1.
C
C             BEGIN OUTER ITERATION LOOP TO UPDATE ALF.
C             CALCULATE THE NORM OF THE RESIDUAL AND THE DERIVATIVE OF
C             THE MODIFIED RESIDUAL THE FIRST TIME, BUT ONLY THE
C             DERIVATIVE IN SUBSEQUENT ITERATIONS.
C
    5 CALL DPA (L, NL, N, NMAX, LPP2, IV, T, Y, W, ALF, ADA, IERR,
     X IPRINT, A, BETA, A(1, LP1), R)
      GNSTEP = 1.0
      ITERIN = 0
      IF (ITER .GT. 0) GO TO 10
         IF (NL .EQ. 0) GO TO 90
         IF (IERR .NE. 1) GO TO 99
C
         IF (IPRINT .LE. 0) GO TO 10
         WRITE (OUTPUT, 207) ITERIN, R
         WRITE (OUTPUT, 200) NU
C                              BEGIN TWO-STAGE ORTHOGONAL FACTORIZATION
   10 CALL ORFAC1(NLP1, NMAX, N, L, IPRINT, A(1, B1), PRJRES, IERR)
      IF (IERR .LT. 0) GO TO 99
      IERR = 2
      IF (NU .EQ. 0.) GO TO 30
C
C             BEGIN INNER ITERATION LOOP FOR GENERATING NEW ALF AND
C             TESTING IT FOR ACCEPTANCE.
C
   25    CALL ORFAC2(NLP1, NMAX, NU, A(1, B1))
C
C             SOLVE A NL X NL UPPER TRIANGULAR SYSTEM FOR DELTA-ALF.
C             THE TRANSFORMED RESIDUAL (IN COL. LNL2 OF A) IS OVER-
C             WRITTEN BY THE RESULT DELTA-ALF.
C
   30    CALL BACSUB (NMAX. NL, A(1, B1), A(1, LNL2))
         DO 35 K = 1, NL
   35       A(K, B1)  = ALF(K) + A(K, LNL2)
```

```
C           NEW ALF(K) = ALF(K) + DELTA ALF(K)
C
C              STEP TO THE NEW POINT NEW ALF, AND COMPUTE THE NEW
C              NORM OF RESIDUAL.  NEW ALF IS STORED IN COLUMN B1 OF A.
C
   40    CALL DPA (L, NL, N, NMAX. LPP2, IV, T, Y, W, A(1, B1), ADA,
     X   IERR, JPRINT, A, BETA, A(1, LP1), RNEW)
         IF (IERR .NE. 2) GO TO 99
         ITER = ITER + 1
         ITERIN = ITERIN + 1
         SKIP = MOD(ITER, MODIT) .NE. O
         IF (SKIP) GO TO 45
            WRITE (OUTPUT. 203) ITER
            WRITE (OUTPUT, 216) (A(K, B1), K = 1, NL)
            WRITE (OUTPUT. 207) ITERIN, RNEW
C
   45    IF (ITER .LT. ITMAX) GO TO 50
            IERR = -1
            CALL VARERR (IPRINT, IERR, 1)
            GO TO 95
   50    IF (RNEW - R .LT. EPS1*(R + 1.DØ)) GO TO 75
C
C              RETRACT THE STEP JUST TAKEN
C
            IF (NU .NE. Ø.) GO TO 60
C                                          GAUSS-NEWTON OPTION ONLY
            GNSTEP = Ø.5*GNSTEP
            IF (GNSTEP .LT. EPS1) GO TO 95
            DO 55 K = 1, NL
   55          A(K, B1) = ALF(K) + GNSTEP*A(K, LNL2)
            GO TO 40
C                                          ENLARGE THE MARQUARDT PARAMETER
   60       NU = 1.5*NU
            IF (.NOT. SKIP) WRITE (OUTPUT. 206) NU
            IF (NU .LE. 1110.) GO TO 65
               IERR = -2
               CALL VARERR (IPRINT, IERR, 1)
               GO TO 95
C                                          RETRIEVE UPPER TRIANGULAR FORM
C                                          AND RESIDUAL OF FIRST STAGE.
   65    DO 70 K = 1, NL
            KSUB = LP1 + K
            DO 70 J = K, NLP1
               JSUB = LP1 + J
               ISUB = NLPI + J
   70          A(K, JSUB) = A(ISUB, KSUB)
         GO TO 25
C                                          END OF INNER ITERATION LOOP
C              ACCEPT THE STEP JUST TAKEN
C
   75 R = RNEW
      DO 80 K = 1, NL
   80    ALF(K) = A(K, B1)
C                                          CALC. NORM(DELTA ALF)/NORM(ALF)
      ACUM = GNSTEP*XNORM(NL, A(1, LNL2))/XNORM(NL, ALF)
C
C              IF ITERIN IS GREATER THAN 1, A STEP WAS RETRACTED DURING
C              THIS OUTER ITERATION.
C
      IF (ITERIN .EQ. 1) NU = Ø.5*NU
      IF (SKIP) GO TO 85
         WRITE (OUTPUT, 2110) NU
         WRITE (OUTPUT, 2118) ACUM
   85 IERR = 3
```

```
      IF (PRJRES .GT. EPS1*(R + 1.DØ)) GO TO 5
C           END OF OUTER ITERATION LOOP
C
C           CALCULATE FINAL QUANTITIES -- LINEAR PARAMETERS, RESIDUALS,
C           COVARIANCE MATRIX, ETC.
C
   90 IERR = ITER
   95 IF (NL .GT. Ø) CALL DPA(L, NL, N, NMAX, LPP2, IV, T. Y, W, ALF,
     X ADA, 4, IPRINT, A, BETA, A(1, LP1), R)
      CALL POSTPR(L, NL, N, NMAX, LNL2, EPS1, R, IPRINT, ALF, W, A,
     X A(1, LP1), BETA, IERR)
   99 RETURN
C
  200 FORMAT (9H      NU =, E15.7)
  203 FORMAT (12HØ  ITERATION, 14, 24H    NONLINEAR PARAMETERS)
  206 FORMAT (25H      STEP RETRACTED, NU =  E15.7)
  207 FORMAT (1HØ, I5, 20H  NORM OF RESIDUAL =, E15.7)
  208 FORMAT (34H      NORM(DELTA-ALF) / NORM(ALF) =, E12.3)
  216 FORMAT (1HØ, 7E15.7)
      END
C
      SUBROUTINE ORFAC1(NLP1, NMAX, N, L, IPRINT, B, PRJRES, IERR)
C
C            STAGE 1:  HOUSEHOLDER REDUCTION OF
C
C                    (          )      ( DR'.  R3 )     NL
C                    ( DR . R2 )  TO   (----, -- ),
C                    (          )      (  O . R4 )  N-L-NL
C
C                      NL    1          NL    1
C
C         WHERE DR = -D(Q2)*Y IS THE DERIVATIVE OF THE MODIFIED RESIDUAL
C         PRODUCED BY DPA, R2 IS THE TRANSFORMED RESIDUAL FROM DPA, AND
C         DR' IS IN UPPER TRIANGULAR FORM (AS IN REF. (2), P. 18).
C         DR IS STORED IN ROWS L+1 TO N AND COLUMNS L+2 TO L + NL + 1 OF
C         THE MATRIX A (I.E., COLUMNS 1 TO NL OF THE MATRIX B).  R2 IS
C         STORED IN COLUMN L + NL + 2 OF THE MATRIX A (COLUMN NL + 1 OF
C         B).  FOR K = 1, 2, ..., NL, FIND REFLECTION I - U * U' / BETA
C         WHICH ZEROES B(I, K), I = L+K+1, ..., N.
C
C     ..................................................................
C
      DOUBLE PRECISION ACUM, ALPHA, B(NMAX, NLP1), BETA. DSIGN, PRJRES,
     X U, XNORM
C
      NL = NLPI - 1
      NL23 = 2*NL + 3
      LP1 = L + 1
C
      DO 30 K = 1, NL
         LPK = L + K
         ALPHA = DSIGN(XNORM(N+1-LPK, B(LPK, K)), B(LPK, K))
         U = B(LPK, K) + ALPHA
         B(LPK, K) = U
         BETA = ALPHA * U
         IF (ALPHA .NE. O.O) GO TO 13
C                                                  COLUMN WAS ZERO
         IERR = -8
         CALL VARERR (IPRINT, IERR, LP1 + K)
         GO TO 99
C                                  APPLY REFLECTIONS TO REMAINING COLUMNS
C                                  OF B AND TO RESIDUAL VECTOR.
   13    KP1 = K + 1
         DO 25 J = KP1, NLPI
```

```
            ACUM = 0.0
            DO 20 I = LPK, N
   20          ACUM = ACUM + B(I, K) * B(I, J)
            ACUM = ACUM / BETA
            DO 25 I = LPK, N
   25          B(I, J) = B(I, J) - B(I, K) * ACUM
   30    B(LPK, K) = -ALPHA
C
      PRJRES = XNORM(NL, B(LP1, NLP1))
C
C           SAVE UPPER TRIANGULAR FORM AND TRANSFORMED RESIDUAL, FOR USE
C           IN CASE A STEP IS RETRACTED.  ALSO COMPUTE COLUMN LENGTHS.
C
      IF (IERR .EQ. 4) GO TO 99
      DO 50 K = 1, NL
         LPK = L + K
         DO 40 J = K, NLPI
            JSUB = NLPI + J
            B(K, J) = B(LPK, J)
   40       B(JSUB, K) = B(LPK, J)
   50    B(NL23, K) = XNORM(K, B(LP1, K)) .                                  5
C
   99 RETURN
      END
C
      SUBROUTINE ORFAC2(NLP1, NMAX, NU, B)
C
C        STAGE 2:  SPECIAL HOUSEHOLDER REDUCTION OF
C
C                       NL      ( DR' . R3 )       (DR'' . R5 )
C                               (----------)       (----------)
C                  N-L-NL       (  0  . R4 )  TO   (  0  . R4 )
C                               (----------)       (----------)
C                       NL      (NU*D . 0  )       (  0  . R6 )
C
C                                  NL    1            NL    1
C
C        WHERE DR', R3, AND R4 ARE AS IN ORFAC1, NU IS THE MARQUARDT
C        PARAMETER, D IS A DIAGONAL MATRIX CONSISTING OF THE LENGTHS OF
C        THE COLUMNS OF DR', AND DR'' IS IN UPPER TRIANGULAR FORM.
C        DETAILS IN (1), PP. 423-424.  NOTE THAT THE (N-L-NL) BAND OF
C        ZEROES, AND R4, ARE OMITTED IN STORAGE.
C
C     ..................................................................
C
      DOUBLE PRECISION ACUM, ALPHA, B(NMAX, NLPI). BETA, DSIGN, NU, U,
     X XNORM
C
      NL = NLPI - 1
      NL2 = 2*NL
      NL23 = NL2 + 3
      DO 30 K = 1. NL
         KP1 = K + 1
         NLPK = NL + K
         NLPKM1 = NLPK - 1
         B(NLPK, K) = NU * B(NL23, K)
         B(NL, K) = B(K, K)
         ALPHA = DSIGN(XNORM(K+1, B(NL, K)), B(K, K))
         U = B(K, K) + ALPHA
         BETA = ALPHA * U
         B(K, K) = -ALPHA
C                        THE K-TH REFLECTION MODIFIES ONLY ROWS K,
C                        NL+1, NL+2, ..., NL+K, AND COLUMNS K TO NL+1.
         DO 30 J = KP1, NLP1
```

```
            B(NLPK, J) = 8.
            ACUM = U * B(K,J)
            DO 20 I = NLP1, NLPKM1
   20          ACUM = ACUM + B(I,K) * B(I,J)
            ACUM = ACUM / BETA
            B(K,J) = B(K,J) - U * ACUM
            DO 30 I = NLP1, NLPK
   30          B(I,J) = B(I,J) - B(I,K) * ACUM
C
      RETURN
      END
C
      SUBROUTINE DPA (L, NL, N. NMAX, LPP2, IV, T. V, W, ALF, ADA, ISEL,
     X IPRINT, A, U, R, RNORM)
C
C        COMPUTE THE NORM OF THE RESIDUAL (IF ISEL = 1 OR 2), OR THE
C        (N-L) X NL DERIVATIVE OF THE MODIFIED RESIDUAL (N-L) VECTOR
C        Q2*Y (IF ISEL = 1 OR 3).  HERE Q * PHI = S, I.E.,
C
C          L     ( Q1 ) (                    )   ( S  . R1 .  F1  )
C                (----) ( PHI . Y . D(PHI) ) = (--- . -- . ---- )
C          N-L   ( Q2 ) (                    )   ( O  . R2 .  F2  )
C
C                   N       L    1      P          L     1     P
C
C        WHERE Q IS N X N ORTHOGONAL, AND S IS L X L UPPER TRIANGULAR.
C        THE NORM OF THE RESIDUAL = NORM(R2), AND THE DESIRED DERIVATIVE
C        ACCORDING TO REF. (5), IS
C                                                    -1
C                     D(Q2 * Y) = -Q2 * D(PHI)* S    * Q1* Y.
C
C     ..................................................................
C
      DOUBLE PRECISION A(NMAX, LPP2), ALF(NL), T(NMAX, IV), W(N), Y(N),
     X ACUM, ALPHA, BETA, RNORM, DSIGN, DSQRT, SAVE, R(N), U(L), XNORM
      INTEGER FIRSTC, FIRSTR, INC(12, 8)
      LOGICAL NOWATE, PHILP1
      EXTERNAL ADA
C
      IF (ISEL .NE. 1) GO TO 3
         LP1 = L + 1
         LNLZ = L + 2 + NL
         LP2 = L + 2
         LPP1 = LPP2 - 1
         FIRSTC = 1
         LASTC = LPP1
         FIRSTR = LP1
         CALL INIT(L, NL, N, NMAX, LPP2, IV, T, W, ALF, ADA, ISEL.
     X   IPRINT. A. INC. NCON. NCONP1, PHILP1, NOWATE)
         IF (ISEL .NE. 1) GO TO 99
         GO TO 30
C
    3 CALL ADA (LP1, NL, N, NMAX, LPP2, IV, A, INC, T, ALF, MINØ(ISEL,
     X 3))
      IF (ISEL .EQ. 2) GO TO 6
C                                                    ISEL = 3 OR 4
      FIRSTC = LP2
      LASTC = LPP1
      FIRSTR = (4 - ISEL)*L + 1
      GO TO 50
C                                                    ISEL = 2
    6 FIRSTC = NCONP1
      LASTC = LP1
      IF (NCON .EQ. Ø) GO TO 30
```

```
      IF (A(1, NCON) .EQ. SAVE) GO TO 30
         ISEL = -7
         CALL VARERR (IPRINT, ISEL, NCON)
         GO TO 99
C                                                    ISEL = 1 OR 2
   30 IF (PHILP1) GO TO 48
         DO 35 I = 1, N
   35       R(I) = Y(I)
         GO TO 50
   40    DO 45 I = 1, N
   45       R(I) = Y(I) - R(I)
C                                                    WEIGHT APPROPRIATE COLUMNS
   50 IF (NOWATE) GO TO 58
      DO 55 I = 1, N
         ACUM = W(I)
         DO 55 J = FIRSTC, LASTC
   55       A(I, J) = A(I, J) * ACUM
C
C           COMPUTE ORTHOGONAL FACTORIZATIONS BV HOUSEHOLDER
C           REFLECTIONS.  IF ISEL = 1 OR 2, REDUCE PHI (STORED IN THE
C           FIRST L COLUMNS OF THE MATRIX A) TO UPPER TRIANGULAR FORM,
C           (Q*PHI = S), AND TRANSFORM Y (STORED IN COLUMN L+1), GETTING
C           Q*V = R.  IF ISEL = 1. ALSO TRANSFORM J = D PHI (STORED IN
C           COLUMNS L+2 THROUGH L+P+1 OF THE MATRIX A). GETTING Q*J = F.
C           IF ISEL = 3 OR 4. PHI HAS ALREADY BEEN REDUCED, TRANSFORM
C           ONLY J.  S, R, AND F OVERWRITE PHI, Y, AND J, RESPECTIVELY,
C           AND A FACTORED FORM OF Q IS SAVED IN U AND THE LOWER
C           TRIANGLE OF PHI.
C
   58 IF (L .EO. Ø) GO TO 75
      DO 70 K = 1, L
         KP1 = K + 1
         IF (ISEL .GE. 3 .OR. (ISEL .EQ. 2 .AND. K .LT.NCONP1)) GO TO 66
         ALPHA = DSIGN(XNORM(N+1-K, A(K, K)), A(K, K))
         U(K) = A(K, K) + ALPHA
         A(K, K) = -ALPHA
         FIRSTC = KP1
         IF (ALPHA .NE. 0.0) GO TO 66
         ISEL = -8
         CALL VARERR (IPRINT, ISEL, K)
         GO TO 99
C                                             APPLY REFLECTIONS TO COLUMNS
C                                             FIRSTC TO LASTC.
   66    BETA = -A(K, K) * U(K)
         DO 70 J = FIRSTC, LASTC
            ACUM = U(K)*A(K, J)
            DO 68 I = KP1, N
   68          ACUM = ACUM + A(I, K)*A(I, J)
            ACUM = ACUM / BETA
            A(K,J) = A(K,J) - U(K)*ACUM
            DO 70 I = KP1, N
   70          A(I, J) = A(I, J) - A(I, K)*ACUM
C
   75 IF (ISEL .GE. 3) GO TO 85
      RNORM = XNORM(N-L, R(LP1))
      IF (ISEL .EO. 2) GO TO 99
      IF (NCON .GT. Ø) SAVE = A(1, NCON)
C
C           F2 IS NOW CONTAINED IN ROWS L+I TO N AND COLUMNS L+2 TO
C           L+P+1 OF THE MATRIX A.  NOW SOLVE THE L X L UPPER TRIANGULAR
C           SYSTEM S*BETA = R1 FOR THE LINEAR PARAMETERS BETA.  BETA
C           OVERWRITES R1.
C
   85 IF (L .GT. Ø) CALL BACSUB (NMAX, L, A, R)
```

```
C
C           MAJOR PART OF KAUFMAN'S SIMPLIFICATION OCCURS HERE.  COMPUTE
C           THE DERIVATIVE OF ETA WITH RESPECT TO THE NONLINEAR
C           PARAMETERS
C
C    T*  D ETA          T    L          D PHI(J)     D PHI(L+1)
C   Q  ---------  =  Q * (SUM BETA(J) ------------ + ----------)  =  F2*BETA
C      D ALF(K)          J=1          D ALF(K)       D ALF(K)
C
C           AND STORE THE RESULT IN COLUMNS L+2 TO L+NL+1.  IF ISEL NOT
C           = 4, THE FIRST L ROWS ARE OMITTED.  THIS IS -D(Q2)*Y.  IF
C           ISEL NOT = 4 THE RESIDUAL R2 = Q2*Y (IN COL. L+1) IS COPIED
C           TO COLUMN L+NL+2.  OTHERWISE ALL OF COLUMN L+1 IS COPIED.
C
      DO 95 I = FIRSTR, N
         IF (L .EQ. NCON) GO TO 95
         M = LP1
         DO 90 K = 1, NL
            ACUM = 0.
            DO 88 J = NCONP1, L
               IF (INC(K, J) .EQ. Ø) GO TO 88
               M = M + 1
               ACIJM = ACUM + A(I, M) * R(J)
   88          CONTINUE
            KSUB = LP1 + K
            IF (INC(K, LP1) .EQ. Ø) GO TO 90
            M = M + 1
            ACUM = ACUM + A(I, M)
   90       A(I, KSUB) = ACUM
   95    A(I, LNL2) = R(I)
C
   99 RETURN
      END
C
      SUBROUTINE INIT(L, NL, N, NMAX, LPP2, IV, T, W, ALF, ADA, ISEL,
     X IPRINT. A, INC, NCON, NCONP1, PHILP1, NOWATE)
C
C        CHECK VALIDITY OF INPUT PARAMETERS, AND DETERMINE NUMBER OF
C        CONSTANT FUNCTIONS.
C
C     .....................................................................
C
      DOUBLE PRECISION A(NMAX, LPP2), ALF(NL), T(NMAX, IV), W(N),
     X DSQRT
      INTEGER OUTPUT, P, INC(12, 8)
      LOGICAL NOWATE, PHILP1
      DATA OUTPUT /6/
C
      LP1 = L + 1
      LNL2 = L + 2 + NL
C                                                CHECK FOR VALID INPUT
      IF (L .GE. 0 .AND. NL .GE. 1 .AND. L+NL .LT. N .AND. LNL2 .LE.
     X LPPE .AND. 2*NL + 3 .LE. NMAX .AND. N .LE. NMAX .AND.
     X IV .GT. 0 .AND. .NOT. (NL .EQ. 0 .AND. L .EQ. Ø)) GO TO 1
         ISEL = -4
         CALL VARERR (IPRINT, ISEL, 1)
         GO TO 99
C
    1 IF (L .EQ. 1 .OR. NL .EQ. Ø) GO TO 3
         DO 2 J = 1, LP1
            DO 2 K = 1, NL
    2          INC(K, J) = 0
C
    3 CALL ADA (LP1, NL, N, NMAX, LPPZ, IV, A, INC, T, ALF, ISEL)
```

```
C
      NOWATE = .TRUE.
      DO 9 I = 1, N
         NOWATE = NOWATE .AND. (W(I) .EQ. 1.Ø)
         IF (W(I) .GE. Ø.) GO TO 9
C                                                    ERROR IN WEIGHTS
         ISEL = -6
         CALL VARERR (IPRINT, ISEL, I)
         GO TO 99
    9    W(I) = DSQRT(W(I))
C
      NCOH = L
      NCONP1 = LP1
      PHILP1 = L .EQ. O
      IF (PHILP1 .OR. NL .EQ. Ø) GO TO 99
C                                     CHECK INC MATRIX FOR VALID INPUT AND
C                                     DETERMINE NUMBER OF CONSTANT FCNS.
      P = O
      DO 11 J = 1, LP1
         IF (P .EQ. Ø) NCONP1 = J
         DO 11 K = 1, NL
            INCKJ = INC(K, J)
            IF (INCKJ .NE. O .AND. INCKJ .NE. 1) GO TO 15
            IF (INCKJ .EQ. 1) P = P + 1
   11       CONTIHUE
C
      NCON = NCONP1 - 1
      IF (IPRINT .GE. Ø) WRITE (OUTPUT, 21Ø) NCON
      IF (L+P+2 .EQ. LPP2) GO TO 20
C                                                 INPUT ERROR IN INC MATRIX
   15 ISEL = -5
      CALL VARERR (IPRINT, ISEL, 1)
      GO TO 99
C                                     DETERMINE IF PHI(L+1) IS IN THE MODEL.
   20 DO 25 K = 1, NL
   25    IF (INC(K, LP1) .EQ. 1) PHILP1 = .TRUE.
C
   99 RETURN
  210 FORMAT (33HØ  NUMBER OF CONSTANT FUNCTIONS =, I4 /)
      END
      SUBROUTINE BACSUB (NMAX, N, A, X)
C
C        BACKSOLVE THE N X N UPPER TRIANGULAR SYSTEM A*X = B.
C        THE SOLUTION X OVERWRITES THE RIGHT SIDE B.
C
      DOUBLE PRECISION A(NMAX, N), X(N), ACUM
C
      X(N) = X(N) / A(N, N)
      IF (N .EQ. 1) GO TO 30
      NP1 = N + 1
      DO 20 IBACK = 2, N
         I = NP1 - IBACK
C           I = N-1, N-2, ..., 2, 1
         IP1 = I + 1
         ACUM = X(I)
         DO 10 J = IP1, N
   10       ACUM = ACUM - A(I,J)*X(J)
   20    X(I) = ACUM / A(I,I)
C
   30 RETURN
      END
      SUBROUTINE POSTPR(L, NL, N, NMAX, LNL2, EPS, RNORM, IPRINT, ALF,
     X W, A, R, U. IERR)
C
```

```
C        CALCULATE RESIDUALS, SAMPLE VARIANCE, AND COVARIANCE MATRIX.
C        ON INPUT, U CONTAINS INFORMATION ABOUT HOUSEHOLDER REFLECTIONS
C        FROM DPA.  ON OUTPUT.  IT CONTAINS THE LINEAR PARAMETERS.
C
      DOUBLE PRECISION A(NMAX, LNL2), ALF(NL), R(N), U(L), W(N), ACUM,
     X EPS, PRJRES, RNORM. SAVE, DABS
      INTEGER OUTPUT
      DATA OUTPUT /6/
C
      LP1 = L + 1
      LPNL = LNL2 - 2
      LNL1 = LPNL + 1
      DO 10 I = 1, N
   10    W(I) = W(I)**2
C
C              UNWIND HOUSEHOLDER TRANSFORMATIONS TO GET RESIDUALS,
C              AND MOVE THE LINEAR PARAMETERS FROM R TO U.
C
      IF (L .EQ. Ø) GO TO 30
      DO 25 KBACK = 1, L
         K = LP1 - KBACK
         KP1 = K + 1
         ACUM = O.
         DO 20 I = KP1, N
   20       ACUM = ACUM + A(I, K) * R(I)
         SAVE = R(K)
         R(K) =  ACUM / A(K, K)
         ACUM = -ACUM / (U(K) * A(K, K))
         U(K) = SAVE
         DO 25 I = KP1, N
   25       R(I) = R(I) - A(I, K)*ACUM
C                                                  COMPUTE MEAN ERROR
   30 ACUM = O.
      DO 35 I = 1. N
   35    ACUM = ACUM + R(I)
      SAVE = ACUM / N
C
C              THE FIRST L COLUMNS OF THE MATRIX HAVE BEEN REDUCED TO
C              UPPER TRIANGULAR FORM IN DPA.  FINISH BY REDUCING ROWS
C              L+I TO N AND COLUMNS L+2 THROUGH L+NL+1 TO TRIANGULAR
C              FORM.  THEN SHIFT COLUMNS OF DERIVATIVE MATRIX OVER ONE
C              TO THE LEFT TO BE ADJACENT TO THE FIRST L COLUMNS.
C
      IF (NL .EQ. Ø) GO TO 45
      CALL ORFAC1(NL+1, NMAX, N, L, IPRINT, A(1, L+2), PRJRES, 4)
      DO 4Ø I = 1, N
         A(I, LNL2) = R(I)
         DO 40 K = LP1, LNL1
   45       A(I, K) = A(I, K+1)
C                                                  COMPUTE COVARIANCE MATRIX
   45 A(1, LNL2) = RNORM
      ACUM = RNORM*RNORM/(N - L - NL)
      A(2, LNL2) = ACUM
      CALL COV(NMAX, LPNL, ACUM, A)
C
      IF (IPRINT .LT. Ø) GO TO 99
      WRITE (OUTPUT. 2Ø9)
      IF (L .GT. Ø) WRITE (OUTPUT. 21Ø) (U(J), J = 1, L)
      IF (NL .GT. Ø) WRITE (OUTPUT, 211) (ALF(K), K = 1, NL)
      WRITE (OUTPUT, 214) RNORM. SAVE, ACUM
      IF (DABS(SAVE) .GT. EPS) WRITE (OUTPUT, 215)
      WRITE (OUTPUT, 2Ø9)
   99 RETURN
C
```

```
  209 FORMAT (1HØ, 5Ø(1H'))
  210 FORMAT (2ØHØ  LINEAR PARAMETERS // (7E15.7))
  211 FORMAT (23HØ  NONLINEAR PARAMETERS // (7E15.7))
  214 FORMAT (21HØ  NORM OF RESIDUAL =, E15.7, 33H EXPECTED ERROR OF OBS
     XERVATIONS =, E15.7, / 39H  ESTIMATED VARIANCE OF OBSERVATIONS =,
     X E15.7 )
  215 FORMAT (95H  WARNING -- EXPECTED ERROR OF OBSERVATIONS IS NOT ZERO
     X.  COVARIANCE MATRIX MAY BE MEANINGLESS. /)
      END
      SUBROUTINE COV(NMAX, N, SIGMA2, A)
C
C            COMPUTE THE SCALED COVARIANCE MATRIX OF THE L + NL
C         PARAMETERS.  THIS INVOLVES COMPUTING
C
C                                  2      -1    -T
C                             SIGMA  *  T    *  T
C
C         WHERE THE (L+NL) X (L+NL) UPPER TRIANGULAR MATRIX T IS
C         DESCRIBED IN SUBROUTINE POSTPR.  THE RESULT OVERWRITES THE
C         FIRST L+NL ROWS AND COLUMNS OF THE MATRIX A.  THE RESULTING
C         MATRIX IS SYMMETRIC.  SEE REF. 7, PP. 67-70, 281.
C
C     ..............................................................
C
      DOUBLE PRECISION A(NMAX, N), SUM, SIGMA2
C
      DO 10 J = 1, N
   10    A(J, J) = 1./A(J, J)
C
C                INVERT T UPON ITSELF
C
      IF (N .EQ. 1) GO TO 70
      NM1 = N - 1
      DO 60 I = 1, NM1
         IP1 = I + 1
         DO 60 J = IP1, N
            JM1 = J - 1
            SUM = O.
            DO 50 M = I, JM1
   50          SUM = SUM + A(I, M) * A(M, J)
   60       A(I, J) = -SUM * A(J, J)
C
C                NOW FORM THE MATRIX PRODUCT
C
   70 DO 90 I = 1, N
         DO 90 J = I, N
            SUM = O.
            DO 80 M = J, N
   8Ø          SUM = SUM + A(I, M) * A(J, M)
            SUM = SUM * SIGMA2
            A(I, J) = SUM
   90       A(J, I) = SUM
C
      RETURN
      END
      SUBROUTINE VARERR (IPRINT, IERR, K)
C
C        PRINT ERROR MESSAGES
C
      INTEGER ERRNO, OUTPUT
      DATA OUTPUT /6/
C
      IF (IPRINT .LT. Ø) GO TO 99
      ERRNO = IABS(IERR)
```

```
      GO TO (1, 2, 99, 4, 5, 6, 7, 8), ERRNO
C
    1 WRITE (OUTPUT, 101)
      GO TO 99
    2 WRITE (OUTPUT, 102)
      GO TO 99
    4 WRITE (OUTPUT, 104)
      GO TO 99
    5 WRITE (OUTPUT, 105)
      GO TO 99
    6 WRITE (OUTPUT, 106) K
      GO TO 99
    7 WRITE (OUTPUT, 107) K
      GO TO 99
    8 WRITE (OUTPUT, 108) K
C
   99 RETURN
  101 FORMAT (46HØ  PROBLEM TERMINATED FOR EXCESSIVE ITERATIONS //)
  102 FORMAT (49HØ  PROBLEM TERMINATED BECAUSE OF ILL-CONDITIONING //)
  104 FORMAT (/ 5ØH INPUT ERROR IN PAR METER L, NL, N, LPP2, OR NMAX. /
  105 FORMAT (68HØ  ERROR -- INC MATRIX IMPROPERLY SPECIFIED, OR DISAGRE
     XES WITH LPP2. /)
  106 FORMAT (19HØ  ERROR -- WEIGHT(, I4, 14H) IS NEGATIVE. /)
  107 FORMAT (28HØ  ERROR -- CONSTANT COLUMN , I3, 37H MUST BE COMPUTED
     XONLY WHEN ISEL = 1.  /)
  108 FORMAT (33HØ  CATASTROPHIC FAILURE -- COLUMN , 14, 28H IS ZERO, SE
     XE DOCUMENTATION. /)
      END
      DOUBLE PRECISION FUNCTION XNORM(N, X)
C
C        COMPUTE THE L2 (EUCLIDEAN) NORM OF A VECTOR, MAKING SURE TO
C        AVOID UNNECESSARY UNDERFLOWS.  NO ATTEMPT IS MADE TO SUPPRESS
C        OVERFLOWS.
C
      DOUBLE PRECISION X(N), RMAX. SUM, TERM, DABS, DSQRT
C
C             FIND LARGEST (IN ABSOLUTE VALUE) ELEMENT
      RMAX = O.
      DO 10 I = 1, N
         IF (DABS(X(I)) .GT. RMAX) RMAX = DABS(X(I))
   10    CONTINUE
C
      SUM = O.
      IF (RMAX .EO. Ø.) GO TO 30
      DO 20 I = 1. N
         TERM = O.
         IF (RMAX + DABS(X(I)) .NE.  RMAX) TERM = X(I)/RMAX
   20    SUM = SUM + TERM*TERM
C
   30 XNORM = RMAX*DSQRT(SUM)
   99 RETURN
      END
```

SAMPLE INPUT

```
  48.5
  1
  0.022
  O
 59
  1
  0.117     0.738
  0.167     1.000
  0.667     1.000
  1.167     1.008
  1.667     0.825
  2.017     0.923
  2.167     1.000
  2.417     0.996
  2.667     1.000
  2.917     0.988
  3.167     0.945
  3.417     0.956
  3.667     0.932
  3.917     0.901
  4.167     0.885
  4.417     0.873
  4.667     0.838
  4.917     0.841
  5.167     0.830
  5.417     0.830
  5.667     0.794
  5.917     0.794
  6.167     0.813
  6.417     0.782
  6.667     0.785
  6.917     0.773
  7.167     0.749
  7.417     0.753
  7.917     0.749
  8.417     0.749
  8.917     0.734
  9.917     0.718
 10.917     0.734
 11.917     0.647
 12.917     0.619
 13.917     0.615
 14.917     0.559
 15.917     0.563
 16.917     0.531
 17.917     0.523
 18.917     0.527
 19.917     0.489
 20.917     0.468
 21.917     0.472
 22.917     0.448
 23.917     0.460
 24.917     0.409
 28.917     0.381
 32.917     0.333
 36.917     0.273
 40.917     0.250
 44.917     0.234
 58.917     0.234
 52.917     0.182
 60.917     0.151
 68.917     8.873
```

76.917	0.105
84.917	0.081
92.917	0.063

**********SAMPLE OUTPUT*********

O INJECTION TIME

48.50
O NUMBER OF NONLINEAR PARAMETERS

1
O INITIAL ESTIMATES OF NONLIN. PARAM.

0.0220
O NUMBER OF LINEAR PARAMETERS

O
O NUMBER OF OBSERVATIONS

59
O NUMBER OF INDEPENDENT VARIABLES

1

	INDEPENDENT VARIABLES	DEPENDENT VARIRBLES
O	0.117	0.730
O	0.167	1.000
O	0.667	1.000
O	1.167	1.000
O	1.667	0.825
O	2.017	0.923
O	2.167	1.000
O	2.417	0.996
O	2.667	1.000
O	2.917	0.988
O	3.167	0.945
O	3.417	0.956
O	3.667	0.932
O	3.917	0.901
O	4.167	0.885
O	4.417	0.873
O	4.667	0.830
O	4.917	0.841
O	5.167	0.830
O	5.417	0.830
O	5.667	0.794
O	5.917	0.794
O	6.167	0.813
O	6.417	0.782
O	6.667	0.785
O	6.917	0.773
O	7.167	0.749
O	7.417	0.753
O	7.917	0.749
O	8.417	0.749
O	8.917	0.734
O	9.917	0.718
O	10.917	0.734
O	11.917	0.647
O	12.917	0.619
O	13.917	0.615
O	14.917	0.559
O	15.917	0.563
O	16.917	0.531
O	17.917	0.523
O	18.917	Ø.527
O	19.917	0.489

0	20.917	0.468
0	21.917	0.472
0	22.917	8.448
0	23.917	0.460
0	24.917	0.409
0	28.917	0.381
0	32.917	0.333
0	36.917	0.273
0	40.917	0.250
0	44.917	0.234
0	48.917	0.234
0	52.917	0.182
0	60.917	0.151
0	68.917	0.073
0	76.917	0.105
0	84.917	0.081
0	92.917	0.063

ØINCIDENCE MATRIX INC(1,1)=

1

```
0    0  NORM OF RESIDUAL =  Ø.1757343e+Ø1
        NU =  Ø.1ØØØØØØe+Ø1
0   ITERATION    1     NONLINEAR PARAMETERS
0  Ø.5151109e-Ø1
0     1  NORM OF RESIDUAL =  Ø.114912Øe+Ø1
        NU =  Ø.5ØØØØØØe+ØØ
        NORM(DELTA-ALF) / NORM(ALF) =   Ø.573e+ØØ
0   ITERATION    2     NONLINEAR PARAMETERS
0  Ø.1Ø24895e+ØØ
0     1  NORM OF RESIDUAL =  Ø.6Ø24982e+ØØ
        NU =  Ø.25ØØØØØe+ØØ
        NORMIDELTA-ALF) / NORM(ALF) =   Ø.497e+ØØ
0   ITERATION    3     NONLINEAR PARAMETERS
0  Ø.151Ø6Ø7e+ØØ
0     1  NORM OF RESIDUAL =  Ø.4143Ø13e+ØØ
        NU =  Ø.125ØØØØe+ØØ
        NORMIDELTA-ALF) / NORM(ALF) =   Ø.322e+ØØ
0   ITERATION    4     NONLINEAR PARAMETERS
0  Ø.1682783e+ØØ
0     1  NORM OF RESIDUAL =  Ø.4Ø3Ø864e+ØØ
        NU =  Ø.625ØØØØe-Ø1
        NORM(DELTA-ALF) / NORM(ALF) =   Ø.1Ø2e+ØØ
0   ITERATION    5     NONLINEAR PARAMETERS
0  Ø.16873Ø9e+ØØ
0     1  NORM OF RESIDUAL =  Ø.4Ø3Ø8Ø5e+ØØ
        NU =  Ø.3125ØØØe-Ø1
        NORMIDELTA-ALF) / NORM(ALF) =   Ø.268e-Ø2
0   ITERATION    6     NONLINEAR PARAMETERS
0  Ø.1687Ø41e+ØØ
0     1  NORM OF RESIDUAL =  Ø.4Ø3Ø8Ø5e+ØØ
        NU =  Ø.15625ØØe-Ø1
        NORM(DELTA-ALF) / NORM(ALF) =   Ø.159e-Ø3
0   ITERATION    7     NONLINEAR PARAMETERS
0  Ø.1687Ø58e+ØØ
0     1  NORM OF RESIDUAL =  Ø.4Ø3Ø8Ø6e+ØØ
        NU =  Ø.78125ØØe-Ø2
        NORMIDELTA-ALF) / NORM(ALF) =   Ø.1Ø2e-Ø4
0   ITERATION    8     NONLINEAR PARAMETERS
0  Ø.1687Ø57e+ØØ
0     1  NORM OF RESIDUAL =  Ø.4Ø3Ø8Ø4e+ØØ
        NU =  Ø.39Ø625Øe-Ø2
        NORMIDELTA-ALF) / NORM(ALF) =   Ø.76Øe-Ø6
Ø'''''''''''''''''''''''''''''''''''''''''''''''''
0   NONLINEAR PARAMETERS

  Ø.1687Ø57e+ØØ
0   NORM OF RESIDUAL =  Ø.4Ø3Ø8Ø4e+ØØ EXPECTED ERROR OF OBSERVATIONS = -Ø.163231Ø9e-Ø2
    ESTIMATED VARIANCE OF OBSERVATIONS =  Ø.28Ø1272e-Ø2
  WARNING -- EXPECTED ERROR OF OBSERVATIONS IS NOT ZERO.   COVARIANCE MATRIX MAY BE MEANINGLES

Ø'''''''''''''''''''''''''''''''''''''''''''''''''
```

ØMEASURMENT TIME	CALCULATED CONCENTRATION
0.117	0.994
0.167	0.992
0.667	0.970
1.167	0.950
1.667	0.932
2.817	0.919
2.167	0.914
2.417	0.906
2.667	0.897
2.917	0.889
3.167	0.881
3.417	0.874
3.667	0.866
3.917	0.858
4.167	0.851
4.417	0.844
4.667	0.837
4.917	0.829
5.167	0.822
5.417	0.816
5.667	0.809
5.917	0.802
6.167	0.796
6.417	0.789
6.667	0.783
6.917	0.776
7.167	0.770
7.417	0.764
7.917	0.752
8.417	0.740
8.917	0.728
9.917	0.706
10.917	0.684
11.917	0.663
12.917	0.643
13.917	0.623
14.917	0.604
15.917	0.586
16.917	0.568
17.917	0.551
18.917	0.534
19.917	0.518
20.917	0.502
21.917	0.487
22.917	0.472
23.917	0.457
24.917	0.443
28.917	0.392
32.917	0.347

36.917	0.308
10.917	0.275
44.917	0.246
48.917	0.221
52.917	0.200
60.917	0.166
68.917	0.139
76.917	0.119
04.917	0.103
92.917	0.091

APPENDIX E: Listing of Programs to Perform Nonlinear Curve Fitting of the Convection-Dispersion Model With a Sample Input and a Corresponding output

```
C          LISTING OF THE CURVEFITTING PROGRAMS FOR THE CONVECTION DISPERSION
C          MODEL CONTINUOUS INJECTON CASE
C
C       ***************************************************************************
C       ***************************************************************************
C                    PROGRAM BEGINS
C       ***************************************************************************
C
C                    MAIN PROGRAM ( PROGRAM CURFIT )
C
C       ***************************************************************************
C
C                    DEFINITION OF THE PARAMETERS
C
C
C                TJ : INJECTION PERIOD
C
C                T(I): TIME STEPS AT WHICH THE CONCENTRATIONS ARE MEASURED
C                      DURING BAKFLOW PERIOD
C
C                C : CONCENTRATIONS CALCULATED BY USING THE OPTIMUM VALUE OF
C                    THE NONLINEAR PARAMETER
C
C       ***************************************************************************
C
C                INPUT DATA ARE STORED IN THE FILE "INFILE"
C
C                OUTPUT ARE STORED IN FILE "OUTFILE"
C
C                VALUES OF THE NONLINEAR PARAMETER AND OTHER STATISTICAL
C
C                INFORMATION OF THE CURFIT ARE DISPLAYED ON THE SCREEN TOO
C
C       ***************************************************************************
C
C
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION Y(100),T(100),ALF(2),BETA(2),W(100),A(100,6)
     *,C(100),INC(3,3)
      EXTERNAL ADA
      COMMON TJ
      OPEN(UNIT=8,FILE='INFILE')
      OPEN(UNIT=9,FILE='OUTFILE')
C
C
C     SET PARAMETERS FOR VARPRO
C
C
      READ(8,*)TJ
      WRITE(9,113)
  113 FORMAT(1H0,10x,'INJECTION TIME'//)
      WRITE(9,*)TJ
        NMAX=100
        LPP2=3
        IPRINT=1
        IV=1
        N=53
        L=0
      DO 1 I=1,N
    1  W(I)=1.0
C
C
```

```
C      READ DATA
C
C
C      NL IS THE NUMBER OF NONLINEAR PARAMETERS
C
C
        READ(8,10) NL
   10    FORMAT(I3)
        WRITE(9,12) NL
   12    FORMAT(1HØ,1ØX,'NUMBER OF NONLINEAR PARAMETERS'//(I3))
C
C
C      INITIAL ESTIMATES OF THE NONLINEAR PARAMETERS
C
C
C
        READ(8,15) ALF(1)
   15    FORMAT(F7.3)
        WRITE(9,2Ø) ALF(1)
   20    FORMAT(1HØ,1ØX,'INITIAL ESTIMATES OF NONLIN. PARAM. '//(F7.3))
C
C
C      L IS THE NUMBER OF LINEAR PARAMETERS
C
C
C
        READ(8,22) L
   22    FORMAT(I3)
        WRITE(9,25) L
   25    FORMAT(1HØ,1ØX,'NUMBER OF LINEAR PARAMETERS'//(I3))
C
C
C      N IS THE NUMBER OF OBSERVATIONS
C
C
C
        READ(8,3Ø) N
   30    FORMAT(I3)
        WRITE(9,35) N
   35    FORMAT(1HØ,1ØX,'NUMBER OF OBSERVATIONS'//(I3))
C
C
C      IV IS THE NUMBER OF INDEPENDENT VERIABLES
C
C
        READ(8,4Ø)IV
   40    FORMAT(I3)
        WRITE(9,45)IV
   45    FORMAT(1HØ,1ØX,'NUMBER OF  INDEPENDENT VARIABLES '//(I3))
C
C
C
C      READ THE TIME AND MEASURED CONCENTRATION DATA T(I) AND Y(I)
C
C
C
        READ(8,55) (T(I),Y(I),I=1,N)
   55    FORMAT(2(F7.3.2X))
        WRITE(9.59)
   59    FORMAT(1HØ,1ØX,'INDEPENDENT VARIABLES '//,2(F7.3,3X))
        WRITE(9,6Ø) (T(I),Y(I),I=1,N)
   60    FORMAT(1HØ,'TIME vs MEASURED CONCENTRATIONS'//,2(F7.3,8X))
C
```

```
C
C
      CALL VARPRO(L,NL,N,NMAX,LPP2,IV,T,Y,W,ADA,A,IPRINT,ALF,BETA,
     *IERR)
      DO 23 I=1,N
      G=ALF(1)*(TJ-T(I))/(2.Ø*DSQRT(TJ+T(I)))
      RESULT=DERF(G)
      C(I)=Ø.5*(1.Ø+RESULT)
   23 CONTINUE
      WRITE(9,26)(T(I),C(I),I=1,N)
   26 FORMAT(1HØ.'TIME VS CALCULATED CONCENTRATION'//2(F7.3.8X))
      STOP
      END
```

```
C
C
C
C       ************************************************************************
C       ************************************************************************
C
C                   SUBROUTINE ADA
C
C       ************************************************************************
C
        SUBROUTINE ADA(L,NL,N,NMAX,LPP2,IV,A,INC,T,ALF,ISEL)
        IMPLICIT REAL*8(A-H,O-Z)
        DIMENSION ALF(2),A(1ØØ,6),T(1ØØ),INC(3,3),B(1ØØ,6),Y(1ØØ)
        COMMON TJ
C
C
C
C       SKIP UNLESS ISEL IS EQUAL TO 1
C
C
C       SET INCIDENCE MATRIX, INC(K,J)=1 IF ALP(K) APPEARS IN PHI(J)
C
        IF(ISEL.EQ.2)GO TO 90
        IF(ISEL.EQ.3)GO TO 165
          INC(1.1 )=1.Ø
          WRITE(9,7Ø) INC(1,1)
   70     FORMAT(1HØ,'INCIDENCE MATRIX INC(1,1)= '//(I3))
C
C     CALCULATION OF THE MATRIX A
C
C     STOKE VALUES OF THE FUNCTION IN COLUMN NUMBER 1 OF  A
C
   90  DO 81 I=1,N
        G=ALF(1)*(TJ-T(I))/(2.Ø*DSQRT(TJ+T(I)))
        RESULT=DERF(G)
        A(I,1)=Ø.5*(1.Ø+RESULT)
   81  CONTINUE
C        WRITE(9,1Ø3)(A(I,1),I=1,N)
C 103     FORMAT(1HØ,'COLUMN #1 OF A(I,J) MATRIX'//(F9.5))
C
C      SKIP CALCULATION OF THE DEIVATIVES IF ISEL-2
C
        IF(ISEL.EQ.2)GO TO 200
C
C      STORE VALUES OF THE DERIVATIVES IN COLUMN NUMBER 2 OF A
C
  165  DO 170 I=1,N
        B(I,1)=DEXP(-ALF(1)**2*(TJ**2-2.Ø*TJ*T(I)+T(I)**2)/(4.Ø*(TJ+T(I))))
        A(I,2)=1./(2.*3.1415**Ø.5)*B(I,1)*(TJ-T(I))/DSQRT(TJ+T(I))
  170  CONTINUE
C      WRITE(9,18Ø)(A(I,2),I=1,N)
C 180    FORMAT(1HØ,'COLUMN #2 OF A(I,J) MATRIX'//(F9.5))
  200  CONTINUE
        RETURN
        END
```

```
      SUBROUTINE VARPRO (L, NL, N. NMAX, LPP2, IV. T, V, W, ADA, A,
     X IPRINT, ALF, BETA, IERR)
C
C           GIVEN A SET OF N OBSERVATIONS. CONSISTING OF VALUES Y(1),
C       Y(2), ..., Y(N) OF A DEPENDENT VARIABLE V, WHERE Y(I)
C       CORRESPONDS TO THE IV INDEPENDENT VARIABLE(S) T(I,1), T(I,2),
C       ..., T(I,IV), VARPRO ATTEMPTS TO COMPUTE A WEIGHTED LEAST
C       SQUARES FIT TO A FUNCTION ETA (THE 'MODEL') WHICH IS A LINEAR
C       COMBINATION
C                                    L
C      ETA(ALF, BETA: T) =          SUM  BETA  * PHI (ALF; T) + PHI   (ALF; T)
C                                   J-1     J      J              L+I
C
C       OF NONLINEAR FUNCTIONS PHI(J) (E.G., A SUM OF EXPONENTIALS AND/
C       OR GAUSSIANS). THAT IS, DETERMINE THE LINEAR PARAMETERS
C       BETA(J) AND THE VECTOR OF NONLINEAR PARAMETERS ALF BY MINIMIZ-
C       ING
C
C                                2     N                                2
C          NORM(RESIDUAL)    =  SUM  W  * (Y  - ETA(ALF, BETA; T ))  .
C                               I=1   I     I                    I
C
C       THE (L+1)-ST TERM IS OPTIONAL, AND IS USED WHEN IT IS DESIRED
C       TO FIX ONE OR MORE OF THE BETA'S (RATHER THAN LET THEM BE
C       DETERMINED). VARPRO REQUIRES FIRST DERIVATIVES OF THE PHI'S.
C
C                                  NOTES:
C
C       A) THE ABOVE PROBLEM IS ALSO REFERRED TO AS 'MULTIPLE
C       NONLINEAR REGRESSION'. FOR USE IN STATISTICAL ESTIMATION,
C       VARPRO RETURNS THE RESIDUALS, THE COVARIANCE MATRIX OF THE
C       LINEAR AND NONLINEAR PARAMETERS, AND THE ESTIMATED VARIANCE OF
C       THE OBSERVATIONS.
C
C       B) AN ETA OF THE ABOVE FORM IS CALLED 'SEPARABLE'. THE
C       CASE OF A NONSEPARABLE ETA CAN BE HANDLED BY SETTING L = O
C       AND USING PHI(L+1).
C
C       C) VARPRO MAY ALSO BE USED TO SOLVE LINEAR LEAST SQUARES
C       PROBLEMS (IN THAT CASE NO ITERATIONS ARE PERFORMED). SET
C       NL = O.
C
C       D) THE MAIN ADVANTAGE OF VARPRO OVER OTHER LEAST SQUARES
C       PROGRAMS IS THAT NO INITIAL GUESSES ARE NEEDED FOR THE LINEAR
C       PARAMETERS. NOT ONLY DOES THIS MAKE IT EASIER TO USE, BUT IT
C       OFTEN LEADS TO FASTER CONVERGENCE.
C
C
C     DESCRIPTION OF PARAMETERS
C
C         L        NUMBER OF LINEAR PARAMETERS BETA (MUST BE .GE. Ø).
C         NL       NUMBER OF NONLINEAR PARAMETERS ALF (MUST BE .GE. Ø).
C         N        NUMBER OF OBSERVATIONS. N MUST RE GREATER THAN L + NL
C                  (I.E., THE NUMBER OF OBSERVATIONS MUST EXCEED THE
C                  NUMBER OF PARAMETERS).
C         IV       NUMBER OF INDEPENDENT VARIABLES T.
C         T        REAL N BY IV MATRIX OF INDEPENDENT VARIABLES. T(I, J)
C                  CONTAINS THE VALUE OF THE I-TH OBSERVATION OF THE J-TH
C                  INDEPENDENT VARIABLE.
C         Y        fl-VECTOR OF OBSERVATIONS, ONE FOR EACH ROW OF T.
C         W        ld-VECTOR OF NONNEGATIVE WEIGHTS. SHOULD BE SET TO 1'S
C                  IF WEIGHTS ARE NOT DESIRED. IF VARIANCES OF THE
C                  INDIVIDUAL OBSERVATIONS ARE KNOWN, W(I) SHOULD BE SET
C                  TO 1./VARIANCE(I).
```

```
C          INC      NL X (L+1) INTEGER INCIDENCE MATRIX.  INC(K, J) = 1 IF
C                   NON-LINEAR PARAMETER ALF(K) APPEARS IN THE J-TH
C                   FUNCTION PHI(J).  (THE PROGRAM SETS ALL OTHER INC(K, J)
C                   TO ZERO.)  IF PHI(L+1) IS INCLUDED IN THE MODEL,
C                   THE APPROPRIATE ELEMENTS OF THE (L+1)-ST COLUMN SHOULD
C                   BE SET TO 1'S.  INC IS NOT NEEDED WHEN L = 0 OR NL = 0.
C                   CAUTION:  THE DECLARED ROW DIMENSION OF INC (IN ADA)
C                   MUST CURRENTLY BE SET TO 12.  SEE 'RESTRICTIONS' BELOW.
C          NMAX     THE DECLARED ROW DIMENSION OF THE MATRICES A AND T.
C                   IT MUST BE AT LEAST MAX(N, 2*NL+3).
C          LPP2     L+P+2, WHERE P IS THE NUMBER OF ONES IN THE MATRIX INC.
C                   THE DECLARED COLUMN DIMENSION OF A MUST BE AT LEAST
C                   LPPE.  (IF L = 0. SET LPP2 = NL+2. IF NL = 0, SET LPP2
C                   L+2.)
C          A        REAL MATRIX OF SIZE MAX(N, 2*NL+3) BY L+P+2.  ON INPUT
C                   IT CONTAINS THE PHI(J)'S AND THEIR DERIVATIVES (SEE
C                   BELOW).  ON OUTPUT, THE FIRST L+NL ROWS AND COLUMNS OF
C                   A WILL CONTAIN AN APPROXIMATION TO THE (WEIGHTED)
C                   COVARIANCE MATRIX AT THE SOLUTION (THE FIRST L ROWS
C                   CORRESPOND TO THE LINEAR PARAMETERS, THE LAST NL TO THE
C                   NONLINEAR ONES), COLUMN L+NL+1 WILL CONTAIN THE
C                   WEIGHTED RESIDUALS (Y - ETA), A(1, L+NL+2) WILL CONTAIN
C                   THE (EUCLIDEAN) NORM OF THE WEIGHTED RESIDUAL, AND
C                   A(2, L+NL+2) WILL CONTAIN AN ESTIMATE OF THE (WEIGHTED)
C                   VARIANCE OF THE OBSERVATIONS, NORM(RESIDUAL)**2/
C                   (N - L - NL).
C          IPRINT   INPUT-INTEGER CONTROLLING PRINTED OUTPUT.  IF IPRINT IS
C                   POSITIVE, THE NONLINEAR PARAMETERS, THE NORM OF THE
C                   RESIDUAL, AND THE MARQUARDT PARAMETER WILL BE OUTPUT
C                   EVERY IPRINT-TH ITERATION (AND INITIALLY. AND AT THE
C                   FINAL ITERATION).  THE LINEAR PARAMETERS WILL BE
C                   PRINTED AT THE FINAL ITERATION.  ANY ERROR MESSAGES
C                   WILL ALSO BE PRINTED.  (IPRINT = 1 IS RECOMMENDED AT
C                   FIRST.)  IF IPRINT = 0. ONLY THE FINAL QUANTITIES WILL
C                   BE PRINTED. AS WELL AS ANY ERROR MESSAGES.  IF IPRINT =
C                   -1, NO PRINTING WILL BE DONE.  THE USER IS THEN
C                   RESPONSIBLE FOR CHECKING THE PARAMETER IERR FOR ERRORS.
C          ALF      NL-VECTOR OF ESTIMATES OF NONLINEAR PARAMETERS
C                   (INPUT).  ON OUTPUT IT WILL CONTAIN OPTIMAL VALUES OF
C                   THE NONLINEAR PARAMETERS.
C          BETA     L-VECTOR OF LINEAR PARAMETERS (OUTPUT ONLY).
C          IERR     INTEGER ERROR FLAG (OUTPUT):
C                   .GT. 0 - SUCCESSFUL CONVERGENCE, IERR IS THE NUMBER OF
C                        ITERATIONS TAKEN.
C                   -1  TERMINATED FOR TOO MANY ITERATIONS.
C                   -2  TERMINATED FOR ILL-CONDITIONING (MAROUARDT
C                        PARAMETER TOO LARGE.)  ALSO SEE IERR = -8 BELOW.
C                   -4  INPUT ERROR IN PARAMETER N, L, NL, LPPE, OR NMAX.
C                   -5  INC MATRIX IMPROPERLY SPECIFIED, OR P DISAGREES
C                        WITH LPP2.
C                   -6  A WEIGHT WAS NEGATIVE.
C                   -7  'CONSTANT' COLUMN WAS COMPUTED MORE THAN ONCE.
C                   -8  CATASTROPHIC FAILURE - A COLUMN OF THE A MATRIX HAS
C                        BECOME ZERO.  SEE 'CONVERGENCE FAILURES' BELOW.
C
C                   (IF IERR .LE. -4, THE LINEAR PARAMETERS, COVARIANCE
C                   MATRIX, ETC. ARE NOT RETURNED.)
C
C     SUBROUTINES REQUIRED
C
C          NINE SUBROUTINES, DPA, ORFAC1, ORFAC2, BACSUB, POSTPR, COV,
C        XNORM, INIT, AND VARERR ARE PROVIDED.  IN ADDITION, THE USER
C        MUST PROVIDE A SUBROUTINE (CORRESPONDING TO THE ARGUMENT ADA)
C        WHICH, GIVEN ALF, WILL EVALUATE THE FUNCTIONS PHI(J) AND THEIR
```

```
C       PARTIAL DERIVATIVES D PHI(J)/D ALF(K), AT THE SAMPLE POINTS
C       T(I).  THIS ROUTINE MUST BE DECLARED 'EXTERNAL' IN THE CALLING
C       PROGRAM.  ITS CALLING SEQUENCE IS
C
C       SUBROUTINE ADA (L+1, NL, N, NMAX. LPPZ, IV, A, INC, T, ALF,
C       ISEL)
C
C          THE USER SHOULD MODIFY THE EXAMPLE SUBROUTINE 'ADA' (GIVEN
C       ELSEWHERE) FOR HIS OWN FUNCTIONS.
C
C          THE VECTOR SAMPLED FUIJCTIONS PHI(J) SHOULD BE STORED IN THE
C       FIRST N ROWS AND FIRST L+I COLUMNS OF THE MATRIX A, I.E.,
C       A(I, J) SHOULD CONTAIN PHI(J, ALF; T(I,1), T(I,2), ...,
C       T(I,IV)), I = 1, .... N: J = 1, ..., L (OR L+1).  THE (L+1)-ST
C       COLUMN OF A CONTAINS PHI(L+1) IF PHI(L+1) IS IN THE MODEL,
C       OTHERWISE IT IS RESERVED FOR WORKSPACE.  THE 'CONSTANT' FUNC-
C       TIONS (THESE ARE FUNCTIONS PHI(J) WHICH DO NOT DEPEND UPON ANY
C       NONLINEAR PARAMETERS ALF. E.G.. T(I)**J) (IF ANY) MUST APPEAR
C       FIRST, STARTING IN COLUMN 1.  THE COLUMN N-VECTORS OF NONZERO
C       PARTIAL DERIVATIVES D PHI(J) / D ALF(K) SHOULD BE STORED
C       SEQUENTIALLY IN THE MATRIX A IN COLUMNS L+2 THROUGH L+P+1.
C       THE ORDER IS
C
C          D PHI(1)   D PHI(2)          D PHI(L)   D PHI(L+1)   D PHI(1)
C          --------, --------, ...,    --------, ----------, --------,
C          D ALF(1)   D ALF(1)          D ALF(1)    D ALF(1)    D ALF(2)
C
C          D PHI(2)          D PHI(L+1)          D PHI(1)          D PHI(L+1)
C          --------, ...,    ----------, ....    ----------, ....  ----------,
C          D ALF(2)           D ALF(2)           D ALF(NL)         D ALF(NL)
C
C       OMITTING COLUMNS OF DERIVATIVES WHICH ARE ZERO, AND OMITTING
C       PHI(L+1) COLUMNS IF PHI(L+1) IS NOT IN THE MODEL.  NOTE THAT
C       THE LINEAR PARAMETERS BETA ARE NOT USED IN THE MATRIX A.
C       COLUMN L+P+2 IS RESERVED FOR WORKSPACE.
C
C       THE CODING OF ADA SHOULD BE ARRANGED SO THAT:
C
C       ISEL = 1  (WHICH OCCURS THE FIRST TIME ADA IS CALLED) MEANS:
C                 A.  FILL IN THE INCIDENCE MATRIX INC
C                 B.  STORE ANY CONSTANT PHI'S IN A.
C                 C.  COMPUTE NONCONSTANT PHI'S AND PARTIAL DERIVA-
C                     TIVES.
C            = 2  MEANS COMPUTE ONLY THE NONCONSTANT FUNCTIONS PHI
C            = 3  MEANS COMPUTE ONLY THE DERIVATIVES
C
C       (WHEN THE PROBLEM IS LINEAR (NL = Ø) ONLY ISEL = 1 IS USED, AND
C       DERIVATIVES ARE NOT NEEDED.)
C
C     RESTRICTIONS
C
C          THE SUBROUTINES DPA, INIT (AND ADA) CONTAIN THE LOCALLY
C       DIMENSIONED MATRIX INC, WHOSE DIMENSIONS ARE CURRENTLY SET FOR
C       MAXIMA OF L+I = 8, NL = 12.  THEY MUST BE CHANGED FOR LARGER
C       PROBLEMS.  DATA PLACED IN ARRAY A IS OVERWRITTEN ('DESTROYED').
C       DATA PLACED IN ARRAYS T, Y AND INC IS LEFT INTACT.  THE PROGRAM
C       RUNS IN UATFIV, EXCEPT WHEN L = O OR NL = O.
C
C          IT IS ASSUMED THAT THE MATRIX PHI(J, ALF: T(I)) HAS FULL
C       COLUMN RANK.  THIS MEANS THAT THE FIRST L COLUMNS OF THE MATRIX
C       A MUST BE LINEARLY INDEPENDENT.
C
C          OPTIONAL NOTE:  AS WILL BE NOTED FROM THE SAMPLE SUBPROGRAM
C       ADA, THE DERIVATIVES D PHI(J)/D ALF(K) (ISEL = 3) MUST BE
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```
C       COMPUTED INDEPENDENTLY OF THE FUNCTIONS PHI(J) (ISEL = 2),
C       SINCE THE FUNCTION VALUES ARE OVERWRITTEN AFTER ADA IS CALLED
C       WITH ISEL = 2.  THIS IS DONE TO MINIMIZE STORAGE, AT THE POS-
C       SIBLE EXPENSE OF SOME RECOMPUTATION (SINCE THE FUNCTIONS AND
C       DERIVATIVES FREQUENTLY HAVE SOME COMMON SUBEXPRESSIONS).  TO
C       REDUCE THE AMOUNT OF COMPUTATION AT THE EXPENSE OF SOME
C       STORAGE, CREATE A MATRIX B OF DIMENSION NMAX BY L+I IN ADA, AND
C       AFTER THE COMPUTATION OF THE PHI'S (ISEL = 2), COPY THE VALUES
C       INTO B.  THESE VALUES CAN THEN BE USED TO CALCULATE THE DERIV-
C       ATIVES (ISEL = 3).  (THIS MAKES USE OF THE FACT THAT WHEN A
C       CALL TO ADA WITH ISEL = 3 FOLLOWS A CALL WITH ISEL = 2, THE
C       ALFS ARE THE SAME.)
C
C          TO CONVERT TO OTHER MACHINES, CHANGE THE OUTPUT UNIT IN THE
C       DATA STATEMENTS IN VARPRO, DPA, POSTPR, AND VARERR.  THE
C       PROGRAM HAS BEEN CHECKED FOR PORTABILITY BY THE BELL LABS PFORT
C       VERIFIER.  FOR MACHINES WITHOUT DOUBLE PRECISION HARDWARE, IT
C       MAY BE DESIRABLE TO CONVERT TO SINGLE PRECISION.  THIS CAN BE
C       DONE BY CHANGING (A) THE DECLARATIONS 'DOUBLE PRECISION' TO
C       'REAL'.  (B) THE PATTERN '.D' TO '.E' IN THE 'DATA' STATEMENT IN
C       VARPRO, (C) DSIGN, DSQRT AND DABS TO SIGN, SQRT AND ABS,
C       RESPECTIVELY, AND (D) DEXP TO EXP IN THE SAMPLE PROGRAMS ONLY.
C
C     NOTE ON INTERPRETATION OF COVARIANCE MATRIX
C
C          FOR USE IN STATISTICAL ESTIMATION (MULTIPLE NONLINEAR
C       REGRESSION) VARPRO RETURNS THE COVARIANCE MATRIX OF THE LINEAR
C       AND NONLINEAR PARAMETERS.  THIS MATRIX WILL BE USEFUL ONLY IF
C       THE USUAL STATISTICAL ASSUMPTIONS HOLD:  AFTER WEIGHTING, THE
C       ERRORS IN THE OBSERVATIONS ARE INDEPENDENT AND NORMALLY DISTRI-
C       BUTED, WITH MEAN ZERO AND THE SAME VARIANCE.  IF THE ERRORS DO
C       NOT HAVE MEAN ZERO (OR ARE UNKNOWN), THE PROGRAM WILL ISSUE A
C       WARNING MESSAGE (UNLESS IPRINT .LT. 0) AND THE COVARIANCE
C       MATRIX WILL NOT BE VALID.  IN THAT CASE, THE MODEL SHOULD BE
C       ALTERED TO INCLUDE A CONSTANT TERM (SET PHI(1) = 1.).
C
C          NOTE ALSO THAT, IN ORDER FOR THE USUAL ASSUMPTIONS TO HOLD,
C       THE OBSERVATIONS MUST ALL BE OF APPROXIMATELY THE SAME
C       MAGNITUDE (IN THE ABSENCE OF INFORMATION ABOUT THE ERROR OF
C       EACH OBSERVATION), OTHERWISE THE VARIANCES WILL NOT BE THE
C       SAME.  IF THE OBSERVATIONS ARE NOT THE SAME SIZE, THIS CAN BE
C       CURED BY WEIGHTING.
C
C          IF THE USUAL ASSUMPTIONS HOLD, THE SQUARE ROOTS OF THE
C       DIAGONALS OF THE COVARIANCE MATRIX A GIVE THE STANDARD ERROR
C       S(I) OF EACH PARAMETER.  DIVIDING A(I,J) BY S(I)*S(J) YIELDS
C       THE CORRELATION MATRIX OF THE PARAMETERS.  PRINCIPAL AXES AND
C       CONFIDENCE ELLIPSOIDS CAN BE OBTAINED BY PERFORMING AN EIGEN-
C       VALUE/EIGENVECTOR ANALYSIS ON A.  ONE SHOULD CALL THE EISPACK
C       PROGRAM TRED2, FOLLOWED BY TQL2 (OR USE THE EISPAC CONTROL
C       PROGRAM).
C
C     CONVERGENCE FAILURES
C
C          IF CONVERGENCE FAILURES OCCUR, FIRST CHECK FOR INCORRECT
C       CODING OF THE SUBROUTINE ADA.  CHECK ESPECIALLY THE ACTION OF
C       ISEL, AND THE COMPUTATION OF THE PARTIAL DERIVATIVES.  IF THESE
C       ARE CORRECT, TRY SEVERAL STARTING GUESSES FOR ALF.  IF ADA
C       IS CODED CORRECTLY, AND IF ERROR RETURNS IERR = -2 OR -8
C       PERSISTENTLY OCCUR, THIS IS A SIGN OF ILL-CONDITIONING, WHICH
C       MAY BE CAUSED BY SEVERAL THINGS.  ONE IS POOR SCALING OF THE
C       PARAMETERS:  ANOTHER IS AN UNFORTUNATE INITIAL GUESS FOR THE
C       PARAMETERS, STILL ANOTHER IS A POOR CHOICE OF THE MODEL.
C
```

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C     ALGORITHM
C
C        THE RESIDUAL R IS MODIFIED TO INCORPORATE, FOR ANY FIXED
C     ALF, THE OPTIMAL LINEAR PARAMETERS FOR THAT ALF.  IT IS THEN
C     POSSIBLE TO MINIMIZE ONLY ON THE NONLINEAR PARAMETERS.  AFTER
C     THE OPTIMAL VALUES OF THE NONLINEAR PARAMETERS HAVE BEEN DETER-
C     MINED, THE LINEAR PARAMETERS CAN BE RECOVERED BY LINEAR LEAST
C     SQUARES TECHNIQUES (SEE REF. 1).
C
C        THE MINIMIZATION IS BY A MODIFICATION OF OSBORNE'S (REF. 3)
C     MODIFICATION OF THE LEVENBERG-MARQUARDT ALGORITHM.  INSTEAD OF
C     SOLVING THE NORMAL EQUATIONS WITH MATRIX
C
C                 T      2
C           (J J + NU  * D),        WHERE  J = D(ETA)/D(ALF),
C
C     STABLE ORTHOGONAL (HOUSEHOLDER) REFLECTIONS ARE USED ON A
C     MODIFICATION OF THE MATRIX
C                                    (   J   )
C                                    (-------) ,
C                                    ( NU*D  )
C
C     WHERE D IS A DIAGONAL MATRIX CONSISTING OF THE LENGTHS OF THE
C     COLUMNS OF J.  THIS MARQUARDT STABILIZATION ALLOWS THE ROUTINE
C     TO RECOVER FROM SOME RANK DEFICIENCIES IN THE JACOBIAN.
C     OSBORNE'S EMPIRICAL STRATEGY FOR CHOOSING THE MARQUARDT PARAM-
C     ETER HAS PROVEN REASONABLY SUCCESSFUL IN PRACTICE.  (GAUSS-
C     NEWTON WITH STEP CONTROL CAN BE OBTAINED BY MAKING THE CHANGE
C     INDICATED BEFORE THE INSTRUCTION LABELED 5).  A DESCRIPTION CAN
C     BE FOUND IN REF. (3), AND A FLOW CHART IN (2), P. 22.
C
C     FOR REFERENCE, SEE
C
C     1.  GENE H. GOLUR AND V. PEREYRA, 'THE DIFFERENTIATION OF
C         PSEUDO-INVERSES AND NONLINEAR LEAST SQUARES PROBLEMS WHOSE'
C         VARIABLES SEPARATE,'  SIAM J. NUMER. ANAL. 10, 413-432
C         (1973).
C     2.  ------, SAME TITLE, STANFORD C.S. REPORT 72-261, FEB. 1972.
C     3.  OSBORNE. MICHAEL R., 'SOME ASPECTS OF NON-LINEAR LEAST
C         SQUARES CALCULATIONS., IN LOOTSMA, ED., 'NUMERICAL METHODS
C         FOR NON-LINEAR OPTIMIZATION,'  ACADEMIC PRESS. LONDON, 1972.
C     4.  KROGH, FRED, 'EFFICIENT IMPLEMENTATION OF A VARIABLE PRO-
C         JECTION ALGORITHM FOR NONLINEAR LEAST SQUARES PROBLEMS,'
C         COMM. ACM 17. PP. 167-169 (MARCH, 1974).
C     5.  KAUFMAN, LINDA, 'A VARIABLE PROJECTION METHOD FOR SOLVING
C         SEPARABLE NONLINEAR LEAST SQUARES PROBLEMS', B.I.T.  15,
C         49-57 (1975).
C     6.  DRAPER, N., AND SMITH, H., APPLIED REGRESSION ANALYSIS,
C         WILEY, N.Y., 1966 (FOR STATISTICAL INFORMATION ONLY).
C     7.  C. LAWSON AND R. HANSON, SOLVING LEAST SQUARES PROBLEMS,
C         PRENTICE-HALL, ENGLEWOOD CLIFFS, N. J., 1974.
C
C                    JOHN BOLSTAD
C                    COMPUTER SCIENCE DEPT.,  SERRA HOUSE
C                    STANFORD UNIVERSITY
C                    JANUARY. 1977
C
C     ..................................................................
C
      DOUBLE PRECISION A(NMAX, LPPZ). BETA(L), ALF(NL), TINMAX, IV),
     2 W(N), Y(N), ACUM, EPSI, GNSTEP, NU, PRJRES, R, RNEW, XNORM
      INTEGER B1, OUTPUT
      LOGICAL SKIP
      EXTERNAL ADA
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      DATA EPSI /1.D-6/, ITMAX /40/, OUTPUT /6/
C
C           THE FOLLOWING TWO PARAMETERS ARE USED IN THE CONVERGENCE
C           TEST:  EPSI IS AN ABSOLUTE AND RELATIVE TOLERANCE FOR THE
C           NORM OF THE PROJECTION OF THE RESIDUAL ONTO THE RANGE OF THE
C           JACOBIAN OF THE VARIABLE PROJECTION FUNCTIONAL.
C           ITMAX IS THE MAXIMUM NUMBER OF FUNCTION AND DERIVATIVE
C           EVALUATIONS ALLOWED.  CAUTION:  EPSI MUST NOT BE
C           SET SMALLER THAN 10 TIMES THE UNIT ROUND-OFF OF THE MACHINE.
C
C-----------------------------------------------------------------      005
CALL LIB MONITOR FROM VARPRO, MAINTENANCE NUMBER 509, DATE 77178        006
C***PLEASE DON'T REMOVE OR CHANGE THE ABOVE CALL.  IT IS YOUR ONLY      088
C***PROTECTION AGAINST YOUR USING AN OUT-OF-DATE OR INCORRECT           009
C***VERSION OF THE ROUTINE. THE LIBRARY MONITOR REMOVES THIS CALL,      01
C***SO IT ONLY OCCURS ONCE, ON THE FIRST ENTRY TO THIS ROUTINE.         011
C-----------------------------------------------------------------      012
      IERR = 1
      ITER = 0
      LP1 = L + 1
      B1 = L + 2
      LNLZ = L + NL + 2
      NLP1 = NL + 1
      SKIP = .FALSE.
      MODIT = IPRINT
      IF (IPRINT .LE. 0) MODIT = ITMAX + 2
      NU = 0.
C               IF GAUSS-NEWTON IS DESIRED REMOVE THE NEXT STATEMENT.
      NU = 1.
C
C               BEGIN OUTER ITERATION LOOP TO UPDATE ALF.
C               CALCULATE THE NORH OF THE RESIDUAL AND THE DERIVATIVE OF
C               THE MODIFIED RESIDUAL THE FIRST TIME, BUT ONLY THE
C               DERIVATIVE IN SUBSEQUENT ITERATIONS.
C
    5 CALL DPA (L, NL, N, NMAX, LPP2, IV, T, Y, W, ALF, ADA, IERR,
     X IPRINT. A, BETA, A(1, LP1), R)
      GNSTEP = 1.0
      ITERIN = 0
      IF (ITER .GT. 0) GO TO 10
         IF (NL .EO. 0) GO TO 90
         IF (IERR .NE. 1) GO TO 99
C
         IF (IPRINT .LE. 0) GO TO 10
         WRITE (OUTPUT, 207) ITERIN, R
         WRITE (OUTPUT, 200) NU
C                                BEGIN TWO-STAGE ORTHOGONAL FACTORIZATION
   10 CALL ORFAC1(NLP1, NMAX. N, L, IPRINT, A(1, B1), PRJRES, IERR)
      IF (IERR .LT. 0) GO TO 99
      IERR = 2
      IF (NU .EO. 0.) GO TO 30
C
C               BEGIN INNER ITERATION LOOP FOR GENERATING NEW ALF AND
C               TESTING IT FOR ACCEPTANCE.
C
   25    CALL ORFAC2(NLP1, NMAX, NU, A(1, B1))
C
C               SOLVE A NL X NL UPPER TRIANGULAR SYSTEM FOR DELTA-ALF.
C               THE TRANSFORMED RESIDUAL (IN COL. LNLZ OF A) IS OVER-
C               WRITTEN BY THE RESULT DELTA-ALF.
C
   30    CALL BACSUB (NMAX, NL, A(1, B1), A(1, LNL2))
         DO 35 K = 1, NL
   35       A(K, B1)  = ALF(K) + A(K, LNL2)
```

```
C            NEW ALF(K) = ALF(K) + DELTA ALF(K)
C
C
C               STEP TO THE NEW POINT NEW ALF, AND COMPUTE THE NEW
C               NORM OF RESIDUAL.  NEW ALF IS STORED IN COLUMN B1 OF A.
C
   40    CALL DPA (L, NL, N, NMAX. LPP2, IV, T, Y, W, A(1, B1), ADA,
     X   IERR, IPRINT, A, BETA, AII, LP1), RNEW)
         IF (IERR .NE. 2) GO TO 99
         ITER = ITER + 1
         ITERIN = ITERIN + 1
         SKIP = MOD(ITER, MODIT) .NE. 0
         IF (SKIP) GO TO 45
            WRITE (OUTPUT. 203) ITER
            WRITE (OUTPUT, 216) (A(K, B1), K = 1, NL)
            WRITE (OUTPUT, 207) ITERIN, RNEW
C
   45    IF (ITER .LT. ITMAX) GO TO 50
            IERR = -1
            CALL VARERR (IPRINT, IERR, 1)
            GO TO 95
   50    IF (RNEW - R .LT. EPS1*(R + 1.D0)) GO TO 75
C
C               RETRACT THE STEP JUST TAKEN
C
            IF (NU .NE. 0.) GO TO 60
C                                                GAUSS-NEWTON OPTION ONLY
            GNSTEP = 0.5*GNSTEP
            IF (GNSTEP .LT. EPS1) GO TO 95
            DO 55 K = 1, NL
   55          A(K, B1) = ALF(K) + GNSTEP*A(K, LNL2)
            GO TO 40
C                                          ENLARGE THE MARQUARDT PARAMETER
   60       NU = 1.5*NU
            IF (.NOT. SKIP) WRITE (OUTPUT. 206) NU
            IF (NU .LE. 180.) GO TO 65
               IERR = -2
               CALL VARERR (IPRINT, IERR, 1)
               GO TO 95
C                                          RETRIEVE UPPER TRIANGULAR FORM
C                                          AND RESIDUAL OF FIRST STAGE.
   65    DO 70 K = 1, NL
            KSUB = LP1 + K
            DO 70 J = K, NLPI
               JSUB = LP1 + J
               ISUB = NLPI + J
   70          A(K, JSUB) = A(ISUB, KSUB)
         GO TO 25
C                                          END OF INNER ITERATION LOOP
C               ACCEPT THE STEP JUST TAKEN
C
   75 R = RNEW
      DO 80 K = 1, NL
   80    ALF(K) = A(K, B1)
C                                          CALC. NORM(DELTA ALF)/NORM(ALF)
      ACUM = GNSTEP*XNORM(NL, A(1, LNL2))/XNORM(NL, ALF)
C
C               IF ITERIN IS GREATER THAN 1, A STEP WAS RETRACTED DURING
C               THIS OUTER ITERATION.
C
      IF (ITERIN .EQ. 1) NU = 0.5*NU
      IF (SKIP) GO TO 85
         WRITE (OUTPUT. 200) NU
         WRITE (OUTPUT, 208) ACUM
   85 IERR = 3
```

```
      IF (PRJRES .GT. EPS1*(R + 1.DØ)) GO TO 5
C           END OF OUTER ITERATION LOOP
C
C           CALCULATE FINAL QUANTITIES -- LINEAR PARAMETERS, RESIDUALS,
C           COVARIANCE MATRIX, ETC.
C
   90 IERR = ITER
   95 IF (NL .GT. Ø) CALL DPA(L, NL, N, NMAX, LPPZ, IV. T. Y, W, ALF,
     X ADA, 4, IPRINT, A, BETA, A(1, LP1), R)
      CALL POSTPR(L, NL, N, NMAX, LNL2, EPS1, R, IPRINT, ALF, W, A,
     X A(1, LP1), BETA, IERR)
   99 RETURN
C
  200 FORMAT (9H      NU =, E15.7)
  203 FORMAT (12HØ  ITERATION, I4, 24H     NONLINEAR PARAMETERS)
  206 FORMAT (25H      STEP RETRACTED, NU =  E15.7)
  207 FORMAT (1HØ, I5, 2ØH  NORM OF RESIDUAL =, E15.7)
  208 FORMAT (34H      NORM(DELTA-ALF) / NORM(ALF) =, E12.3)
  216 FORMAT (1HØ, 7E15.7)
      END
C
      SUBROUTINE ORFAC1(NLP1, NMAX, N, L, IPRINT, B, PRJRES, IERR)
C
C            STAGE 1:  HOUSEHOLDER REDUCTION OF
C
C                    (     .     )      ( DR'. R3 )    NL
C                    ( DR . R2 )  TO   (----. -- ),
C                    (           )      (  O . R4 )  N-L-NL
C
C                      NL    1           NL    1
C
C          WHERE DP, = -D(Q2)*Y IS THE DERIVATIVE OF THE MODIFIED RESIDUAL
C          PRODUCED BY DPA, R2 IS THE TRANSFORMED RESIDUAL FROM DPA, AND'
C          DR' IS IN UPPER TRIANGULAR FORM (AS IN REF. (2), P. 18).
C          DR IS STORED IN ROWS L+1 TO N AND COLUMNS L+2 TO L + NL + 1 OF
C          THE MATRIX A (I.E., COLUMNS 1 TO NL OF THE MATRIX B).  R2 IS
C          STORED IN COLUMN L + NL + 2 OF THE MATRIX A (COLUMN NL + 1 OF
C          B).  FOP, K = 1, 2, ..., NL. FIND REFLECTION I - U * U' / BETA
C          WHICH ZEROES B(I, K), I = L+K+1, ..., N.
C
C     ..................................................................
C
      DOUBLE PRECISION ACUM, ALPHA, B(NMAX, NLP1), BETA, DSIGN, PRJRES,
     X U, XNORM
C
      NL = NLPI - 1
      NL23 = 2*NL + 3
      LP1 = L + 1
C
      DO 30 K = 1. NL
         LPK = L + K
         ALPHA = DSIGN(XNORM(N+1-LPK, B(LPK, K)), B(LPK, K))
         U = B(LPK, K) + ALPHA
         B(LPK, K) = U
         BETA = ALPHA * U
         IF (ALPHA .NE. O.O) GO TO 13
C                                                  COLUMN WAS ZERO
         IERR = -8
         CALL VARERR (IPRINT, IERR, LP1 + K)
         GO TO 99
C                                 APPLY REFLECTIONS TO REMAINING COLUMNS
C                                 OF B AND TO RESIDUAL VECTOR.
   13    KP1 = K + 1
         DO 25 J = KP1, NLPI
```

```
            ACUM = 0.0
            DO 20 I = LPK, N
   20          ACUM = ACUM + B(I, K) * B(I, J)
            ACUM = ACUM / BETA
            DO 25 I = LPK, N
   25          B(I, J) = B(I, J) - B(I, K) * ACUM
   30    B(LPK, K) = -ALPHA
C
      PRJRES = XNORM(NL, B(LP1, NLP1))
C
C           SAVE UPPER TRIANGULAR FORM AND TRANSFORMED RESIDUAL, FOR USE
C           IN CASE A STEP IS RETRACTED.  ALSO COMPUTE COLUMN LENGTHS.
C
      IF (IERR .EQ. 4) GO TO 99
      DO 50 K = 1, NL
         LPK = L + K
         DO 40 J = K, NLPI
            JSUB = NLPI + J
            B(K, J) = B(LPK, J)
   40       B(JSUB, K) = B(LPK, J)
   58    B(NL23, K) = XNORM(K, B(LP1, K))                                5
C
   99 RETURN
      END
C
      SUBROUTINE ORFAC2(NLP1, NMAX, NU, B)
C
C        STAGE 2:   SPECIAL HOUSEHOLDER REDUCTION OF
C
C                      NL      ( DR' . R3 )       (DR'' . R5 )
C                              (----- -- I        (-----. -- )
C                  N-L-NL      (  Ø  . R4 )  TO   (  O  . R4 )
C                              (----- -- )             . -- )
C                      NL      (NU*D . O  )       (  O  . R6 )
C
C                                NL     1            NL     1
C
C        WHERE DR', R3, AND R4 ARE AS IN ORFAC1, NU IS THE MARQUARDT
C        PARAMETER, D IS A DIAGONAL MATRIX CONSISTING OF THE LENGTHS OF
C        THE COLUMNS OF DR', AND DR'' IS IN UPPER TRIANGULAR FORM.
C        DETAILS IN (1), PP. 423-424.  NOTE THAT THE (N-L-NL) BAND OF
C        ZEROES, AND R4, ARE OMITTED IN STORAGE.
C
C     ..................................................................
C
      DOUBLE PRECISION ACUM. ALPHA, B(NMAX, NLP1), BETA, DSIGN, NU, U,
     X XNORM
C
      NL = NLPI - 1
      NL2 = 2*NL
      NL23 = NL2 + 3
      DO 30 K = 1, NL
         KP1 = K + 1
         NLPK = NL + K
         NLPKM1 = NLPK - 1
         B(NLPK, K) = NU * B(NL23, K)
         B(NL, K) = B(K, K)
         ALPHA = DSIGN(XNORM(K+1, B(NL, K)), B(K, K))
         U = B(K, K) + ALPHA
         BETA = ALPHA * U
         B(K, K) = -ALPHA
C                       THE K-TH REFLECTION MODIFIES ONLY ROWS K,
C                       NL+1, NL+2, ..., NL+K, AND COLUMNS K TO NL+1.
         DO 30 J = KP1, NLPI
```

```
            B(NLPK, J) = Ø.
            ACUM = U * B(K,J)
            DO 20 I = NLP1, NLPKM1
   20          ACUM = ACUM + B(I,K) * B(I,J)
            ACUM = ACUM / BETA
            B(K,J) = B(K,J) - U * ACUM
            DO 30 I = NLP1, NLPK
   30          B(I,J) = B(I,J) - B(I,K) * ACUM
C
      RETURN
      END
C
      SUBROUTINE DPA (L, NL, N, NMAX, LPP2, IV, T, Y, W, ALF, ADA, ISEL,
     X IPRINT. A, U, R, RNORM)
C
C        COMPUTE THE NORM OF THE RESIDUAL (IF ISEL = 1 OR 2), OR THE
C        (N-L) X NL DERIVATIVE OF THE MODIFIED RESIDUAL (N-L) VECTOR
C        Q2*Y (IF ISEL = 1 OR 3).  HERE Q * PHI = S, I.E.,
C
C          L     ( Q1 ) (                    )   ( S  . R1 .  F1  )
C                (----) ( PHI . Y . D(PHI) ) = (--- . -- . ---- )
C          N-L   ( Q2 ) (                    )   ( Ø  . R2 .  F2  )
C
C                  N       L    1      P          L     1     P
C
C        WHERE Q IS N X N ORTHOGONAL, AND S IS L X L UPPER TRIANGULAR.
C        THE NORM OF THE RESIDUAL = NORM(R2), AND THE DESIRED DERIVATIVE
C        ACCORDING TO REF. (5), IS
C                                                          -1
C                    D(Q2 * Y) = -Q2 * D(PHI)* S  * Q1* Y.
C
C     ..................................................................
C
      DOUBLE PRECISION A(NMAX, LPP2), ALF(NL), T(NMAX, IV), W(N), Y(N),
     X ACUM, ALPHA, BETA, RNORM, DSIGN, DSQRT, SAVE, R(N), U(L), XNORM
      INTEGER FIRSTC, FIRSTR, INC(12, 8)
      LOGICAL NOWATE, PHILPI
      EXTERNAL ADA
C
      IF (ISEL .NE. 1) GO TO 3
         LP1 = L + 1
         LNLZ = L + 2 + NL
         LP2 = L + 2
         LPPI = LPPZ - 1
         FIRSTC = 1
         LASTC = LPPI
         FIRSTR = LP1
         CALL INIT(L, NL, N, NMAX, LPP2, IV, T, W, ALF, ADA, ISEL.
     X   IPRINT, A, INC, NCON, NCONPI, PHILPI, NOWATE)
         IF (ISEL .NE. 1) GO TO 99
         GO TO 30
C
    3 CALL ADA (LP1, NL, N, NMAX, LPP2, IV, A, INC, T, ALF, MINØ(ISEL,
     X 3))
      IF (ISEL .EQ. 2) GO TO 6
C                                                    ISEL = 3 OR 4
      FIRSTC = LP2
      LASTC = LPPI
      FIRSTR = (4 - ISEL)*L + 1
      GO TO 50
C                                                    ISEL = 2
    6 FIRSTC = NCONPI
      LASTC = LP1
      IF (NCON .EQ. Ø) GO TO 30
```

```
      IF (A(1, NCON) .EQ. SAVE) GO TO 30
         ISEL = -7
         CALL VARERR (IPRINT, ISEL, NCON)
         GO TO 99
C                                                    ISEL = 1 OR 2
   30 IF (PHILP1) GO TO 48
         DO 35 I = 1, N
   35       R(I) = Y(I)
         GO TO 50
   40    DO 45 I = 1, N
   45       R(I) = Y(I) - R(I)
C                                                    WEIGHT APPROPRIATE COLUMNS
   50 IF (NOWATE) GO TO 58
      DO 55 I = 1, N
         ACUM = W(I)
         DO 55 J = FIRSTC, LASTC
   55       A(I, J) = A(I, J) * ACUM
C
C           COMPUTE ORTHOGONAL FACTORIZATIONS BY HOUSEHOLDER
C           REFLECTIONS.  IF ISEL = 1 OR 2, REDUCE PHI (STORED IN THE
C           FIRST L COLUMNS OF THE MATRIX A) TO UPPER TRIANGULAR FORM,
C           (Q*PHI = S), AND TRANSFORM Y (STORED IN COLUMN L+1), GETTING
C           Q*Y = R.  IF ISEL = 1. ALSO TRANSFORM J = D PHI (STORED IN
C           COLUMNS L+2 THROUGH L+P+1 OF THE MATRIX A), GETTING Q*J = F.
C           IF ISEL = 3 OR 4. PHI HAS ALREADY BEEN REDUCED, TRANSFORM
C           ONLY J.  S, R, AND F OVERWRITE PHI, Y. AND J, RESPECTIVELY,
C           AND A FACTORED FORM OF Q IS SAVED IN U AND THE LOWER
C           TRIANGLE OF PHI.
C
   58 IF (L .EQ. Ø) GO TO 75
      DO 70 K = 1. L
         KP1 = K + 1
         IF (ISEL .GE. 3 .OR. (ISEL .EQ. 2 .AND. E .LT.NCONP1)) GO TO 66
         ALPHA = DSIGN(XNORM(N+1-K, A(K, K)), A(K, K))
         U(K) = A(K, K) + ALPHA
         A(K, K) = -ALPHA
         FIRSTC = KPI
         IF (ALPHA .NE. 0.0) GO TO 66
         ISEL = -8
         CALL VARERR (IPRINT, ISEL, K)
         GO TO 99
C                                          APPLY REFLECTIONS TO COLUMNS
C                                          FIRSTC TO LASTC.
   66    BETA = -A(K, K) * U(K)
         DO 70 J = FIRSTC, LASTC
            ACUM = U(K)*A(K, J)
            DO 68 I = KP1, N
   68          ACUM = ACUM + A(I, K)*A(I, J)
            ACUM = ACUM / BETA
            A(K,J) = A(K,J) - U(K)*ACUM
            DO 70 I = KP1, N
   70          A(I, J) = A(I, J) - A(I, K)*ACUM
C
   75 IF (ISEL .GE. 3) GO TO 85
      RNORM = XNORM(N-L, R(LP1))
      IF (ISEL .EQ. 2) GO TO 99
      IF (NCON .GT. Ø) SAVE = A(1, NCON)
C
C           F2 IS NOW CONTAINED IN ROWS L+I TO N AND COLUMNS L+2 TO
C           L+P+1 OF THE MATRIX A.  NOW SOLVE THE L X L UPPER TRIANGULAR
C           SYSTEM S*BETA = R1 FOR THE LINEAR PARAMETERS BETA.  BETA
C           OVERWRITES R1.
C
   85 IF (L .GT. Ø) CALL BACSUB (NMAX. L, A, R)
```

```
C
C           MAJOR PART OF KAUFMAN'S SIMPLIFICATION OCCURS HERE.  COMPUTE
C           THE DERIVATIVE OF ETA WITH RESPECT TO THE NONLINEAR
C           PARAMETERS
C
C        D  TA          T    L          D PHI(J)    D PHI(L+1)
C  Q * --------  =  Q *  (SUM BETA(J) --------  +  ----------- )  =  F2*BETA
C      D ALF(K)          J=1          D ALF(K)      D ALF(K)
C
C           AND STORE THE RESULT IN COLUMNS L+2 TO L+NL+1.  IF ISEL NOT
C           = 4, THE FIRST L ROWS ARE OMITTED.  THIS IS -D(Q2)*Y.  IF
C           ISEL NOT = 4 THE RESIDUAL R2 = Q2*Y (IN COL. L+1) IS COPIED
C           TO COLUMN L+NL+2.  OTHERWISE ALL OF COLUMN L+1 IS COPIED.
C
      DO 95 I = FIRSTR, N
         IF (L .EO. NCON) GO TO 95
         M = LP1
         DO 90 K = 1, NL
            ACUM = O.
            DO 88 J = NCONP1 , L
               IF (INC(K, J) .EQ. Ø) GO TO 88
               M = M + 1
               ACUM = ACUM + A(I, M) * R(J)
   88          CONTINUE
            KSUB = LP1 + K
            IF (INC(K, LP1) .EQ. Ø) GO TO 90
            M = M + 1
            ACUM = ACUM + A(I, M)
   90       A(I, KSUB) = ACUM
   95    A(I, LNLZ) = R(I)
C
   99 RETURN
      END
C
      SUBROUTINE INIT(L, NL, N, NMAX, LPP2, IV, T, W, ALF. ADA, ISEL,
     X IPRINT, A, INC, NCON, NCONP1, PHILPI, NOWATE)
C
C        CHECK VALIDITY OF INPUT PARAMETERS, AND DETERMINE NUMBER OF
C        CONSTANT FUNCTIONS.
C
C     ..................................................................
C
      DOUBLE PRECISION A(NMAX, LPP2), ALF(NL), T(NMAX, IV), W(N),
     X DSQRT
      INTEGER OUTPUT, P, INC(12, 8)
      LOGICAL NOWATE, PHILPI
      DATA OUTPUT /6/
C
      LP1 = L + 1
      LNL2 = L + 2 + NL
C                                          CHECK FOR VALID INPUT
      IF (L .GE. Ø .AND. NL .GE. Ø .AND. L+NL .LT. N .AND. LNL2 .LE.
     X LPP2 .AND. 2*NL + 3 .LE. NMAX .AND. N .LE. NMAX .AND.
     X IV .GT. O .AND. .NOT. (NL .EQ. O .AND. L .EQ. Ø)) GO TO 1
         ISEL = -4
         CALL VARERR (IPRINT, ISEL, 1)
         GO TO 99
C
    1 IF (L .EQ. Ø .OR. NL .EQ. Ø) GO TO 3
         DO 2 J = 1. LP1
            DO 2 K = 1, NL
    2          INC(K, J) = Ø
C
    3 CALL ADA (LP1, NL, N, NMAX, LPP2, IV, A, INC, T, ALF, ISEL)
```

```
C
      NOWATE = .TRUE.
      DO 9 I = 1, N
         NOWATE = NOWATE .AND. (W(I) .EQ. 1.Ø)
         IF (W(I) .GE. Ø.) GO TO 9
C                                                    ERROR IN WEIGHTS
         ISEL = -6
         CALL VARERR (IPRINT, ISEL, I)
         GO TO 99
    9    W(I) = DSQRT(W(I))
C
      NCOH = L
      NCONP1 = LP1
      PHILP1 = L .EQ. O
      IF (PHILP1 .OR. NL .EQ. Ø) GO TO 99
C                                    CHECK INC MATRIX FOR VALID INPUT AND
C                                    DETERMINE NUMBER OF CONSTANT FCNS.
      P = Ø
      DO 11 J = 1, LP1
         IF (P .EQ. Ø) NCONP1 = J
         DO 11 K = 1, NL
            INCKJ = INC(K, J)
            IF (INCKJ .NE. O .AND. INCKJ .NE. 1) GO TO 15
            IF (INCKJ .EQ. 1) P = P + 1
   11       CONTINUE
C
      NCON = NCONP1 - 1
      IF (IPRINT .GE. Ø) WRITE (OUTPUT, 21Ø) NCON
      IF (L+P+2 .EQ. LPP2) GO TO 20
C                                                INPUT ERROR IN INC MATRIX
   15 ISEL = -5
      CALL VARERR (IPRINT. ISEL. 1)
      GO TO 99
C                                    DETERMINE IF PHI(L+1) IS IN THE MODEL.
   20 DO 25 K = 1, NL
   25    IF (INC(K, LP1) .EQ. 1) PHILP1 = .TRUE.
C
   99 RETURN
  21Ø FORMAT (33HØ  NUMBER OF CONSTANT FUNCTIONS =, I4 /)
      END
      SUBROUTINE BACSUB (NMAX, N, A, X)
C
C        BACKSOLVE THE N X N UPPER TRIANGULAR SYSTEM A*X = B.
C        THE SOLUTION X OVERWRITES THE RIGHT SIDE B.
C
      DOUBLE PRECISION A(NMAX, N), X(N), ACUM
C
      X(N) = X(N) / A(N, N)
      IF IN .EQ. 1) GO TO 30
      NP1 = N + 1
      DO 2Ø IBACK = 2, N
         I = NP1 - IBACK
C           I = N-1, N-2, ..., 2, 1
         IP1 = I + 1
         ACUM = X(I)
         DO 1O J = IP1, N
   1O       ACUM = ACUM - A(I,J)*X(J)
   20    X(I) = ACUM / A(I,I)
C
   30 RETURN
      END
      SUBROUTINE POSTPR(L, NL, N, NMAX, LNL2, EPS, RNORM, IPRINT, ALF,
     X W, A, R, U. IERR)
C
```

```
C         CALCULATE RESIDUALS, SAMPLE VARIANCE, AND COVARIANCE MATRIX.
C         ON INPUT, U CONTAINS INFORMATION ABOUT HOUSEHOLDER REFLECTIONS
C         FROM DPA.  ON OUTPUT, IT CONTAINS THE LINEAR PARAMETERS.
C
      DOUBLE PRECISION A(NMAX, LNL2), ALF(NL), R(N), U(L), W(N), ACUM,
     X EPS, PRJRES, RNORM, SAVE, DABS
      INTEGER OUTPUT
      DATA OUTPUT /6/
C
      LP1 = L + 1
      LPNL = LNLZ - 2
      LNL1 = LPNL + 1
      DO 10 I = 1, N
   10    W(I) = W(I)**2
C
C               UNWIND HOUSEHOLDER TRANSFORMATIONS TO GET RESIDUALS,
C               AND MOVE THE LINEAR PARAMETERS FROM R TO U.
C
      IF (L .EQ. 0) GO TO 38
      DO 25 KBACK = 1, L
         K = LP1 - KBACK
         KP1 = K + 1
         ACUM = 0.
         DO 20 I = KP1, N
   20       ACUM = ACUM + A(I, K) * R(I)
         SAVE = R(K)
         R(K) =  ACUM / A(K, K)
         ACUM = -ACUM / (U(K) * A(K, K))
         U(K) = SAVE
         DO 25 I = KP1, N
   25       R(I) = R(I) - A(I, K)*ACUM
C                                                  COMPUTE MEAN ERROR
   30 ACUM = 0.
      DO 35 I = 1, N
   35    ACUM = ACUM + R(I)
      SAVE = ACUM / N
C
C               THE FIRST L COLUMNS OF THE MATRIX HAVE BEEN REDUCED TO
C               UPPER TRIANGULAR FORM IN DPA.  FINISH BY REDUCING ROWS
C               L+1 TO N AND COLUMNS L+2 THROUGH L+NL+1 TO TRIANGULAR
C               FORM.  THEN SHIFT COLUMNS OF DERIVATIVE MATRIX OVER ONE
C               TO THE LEFT TO BE ADJACENT TO THE FIRST L COLUMNS.
C
      IF (NL .EQ. 0) GO TO 45
      CALL ORFAC1(NL+1, NMAX, N, L, IPRINT, A(1, L+2), PRJRES, 4)
      DO 40 I = 1, N
         A(I, LNL2) = R(I)
         DO 40 K = LP1, LNL1
   40       A(I, K) = A(I, K+1)
C                                                  COMPUTE COVARIANCE MATRIX
   45 A(1, LNL2) = RNORM
      ACUM = RNORM*RNORM/(N - L - NL)
      A(2, LNL2) = ACUM
      CALL COV(NMAX, LPNL, ACUM, A)
C
      IF (IPRINT .LT. 0) GO TO 99
      WRITE (OUTPUT, 209)
      IF (L .GT. 0) WRITE (OUTPUT. 210) (U(J), J = 1, L)
      IF (NL .GT. 0) WRITE (OUTPUT, 211) (ALF(K), K = 1, NL)
      WRITE (OUTPUT, 214) RNORM, SAVE, ACUM
      IF (DABS(SAVE) .GT. EPS) WRITE (OUTPUT, 215)
      WRITE (OUTPUT, 209)
   99 RETURN
C
```

```
  209 FORMAT (1HØ, 5Ø(1H'))
  210 FORMAT (2ØHØ  LINEAR PARAMETERS // (7E15.7))
  211 FORMAT (23HØ  NONLINEAR PARAMETERS // (7E15.7))
  214 FORMAT (21HØ  NORM OF RESIDUAL =, E15.7,  33H EXPECTED ERROR OF OSS
     XERVATIONS =, E15.7,  / 39H   ESTIMATED VARIANCE OF OBSERVATIONS =,
     X E15.7  )
  215 FORMAT (95H  WARNING -- EXPECTED ERROR OF OBSERVATIONS IS NOT ZERO
     X.  COVARIANCE MATRIX MAY BE MEANINGLESS. /)
      END
      SUBROUTINE COV(NMAX, N, SIGMA2, A)
C
C          COMPUTE THE SCALED COVARIANCE MATRIX OF THE L + NL
C       PARAMETERS.  THIS INVOLVES COMPUTING
C
C                                2     -1    -T
C                          SIGMA  *  T   * T
C
C       WHERE THE (L+NL) X (L+NL) UPPER TRIANGULAR MATRIX T IS
C       DESCRIBED IN SUBROUTINE POSTPR.  THE RESULT OVERWRITES THE
C       FIRST L+NL ROWS AND COLUMNS OF THE MATRIX A.  THE RESULTING
C       MATRIX IS SYMMETRIC.  SEE REF. 7, PP. 67-70, 281.
C
C     ..................................................................
C
      DOUBLE PRECISION A(NMAX, N), SUM, SIGMA2
C
      DO 10 J = 1, N
   10    A(J, J) = 1./A(J, J)
C
C                 INVERT T UPON ITSELF
C
      IF (N .EQ. 1) GO TO 70
      NM1 = N - 1
      DO 6Ø I = 1. NMI
         IP1 = I + 1
         DO 60 J = IP1, N
            JM1 = J - 1
            SUM = O.
            DO 50 M = I, JM1
   50          SUM = SUM + A(I, M) * A(M, J)
   6Ø       A(I, J) = -SUM * A(J, J)
C
C                 NOW FORM THE MATRIX PRODUCT
C
   70 DO 90 I = 1. N
         DO 90 J = I, N
            SUM = O.
            DO 80 M = J, N
   80          SUM = SUM + A(I, M) * A(J, M)
            SUM = SUM * SIGMA2
            A(I, J) = SUM
   90       A(J, I) = SUM
C
      RETURN
      END
      SUBROUTINE VARERR (IPRINT, IERR, K)
C
C        PRINT ERROR MESSAGES
C
      INTEGER ERRNO, OUTPUT
      DATA OUTPUT /6/
C
      IF (IPRINT .LT. Ø) GO TO 99
      ERRNO = IABS(IERR)
```

```
      GO TO (1, 2, 99, 4, 5, 6, 7, 8), ERRNO
C
    1 WRITE (OUTPUT, 101)
      GO TO 99
    2 WRITE (OUTPUT, 102)
      GO TO 99
    4 WRITE (OUTPUT, 104)
      GO TO 99
    5 WRITE (OUTPUT, 105)
      GO TO 99
    6 WRITE (OUTPUT, 106) K
      GO TO 99
    7 WRITE (OUTPUT, 107) K
      GO TO 99
    8 WRITE (OUTPUT, 108) K
C
   99 RETURN
  101 FORMAT (46HØ  PROBLEM TERMINATED FOR EXCESSIVE ITERATIONS //)
  102 FORMAT (49HØ  PROBLEM TERMINATED BECAUSE OF ILL-CONDITIONING //)
  104 FORHAT (/ 50H INPUT ERROR IN PARAMETER L. NL, N. LPPZ, OR NMAX. /)
  105 FORMAT (68HØ  ERROR -- INC MATRIX IMPROPERLY SPECIFIED, OR DISAGRE
     XES WITH LPP2. /)
  106 FORMAT (19HØ  ERROR -- WEIGHT(, I4, 14H) IS NEGATIVE. /)
  107 FORHAT (28HØ  ERROR -- CONSTANT COLUMN , I3, 37H MUST BE COMPUTED
     XONLY WHEN ISEL = 1.  /)
  108 FORHAT (33HØ  CATASTROPHIC FAILURE -- COLUMN , I4, 28H IS ZERO, SE
     XE DOCUMENTATION. /)
      END
      DOUBLE PRECISION FUNCTION XNORM(N, X)
C
C        COMPUTE THE L2 (EUCLIDEAN) NORM OF A VECTOR, MAKING SURE TO
C        AVOID UNNECESSARY UNDEKFLOWS.  NO ATTEMPT IS MADE TO SUPPRESS
C        OVERFLOWS.
C
      DOUBLE PRECISION X(N), RMAX. SUM, TERM, DABS, DSQRT
C
C            FIND LARGEST (IN ABSOLUTE VALUE) ELEMENT
      RMAX = O.
      DO 10 I = 1, N
         IF (DABS(X(I)) .GT. RMAX) RMAX = DABS(X(I))
   10    CONTINUE
C
      SUM = Ø.
      IF IRMAX .EQ. Ø.) GO TO 30
      DO 20 I = 1. N
         TERM = O.
         IF (RMAX + DABS(X(I)) .NE. RMAX) TERM = X(I)/RMAX
   20    SUM = SUM + TERM*TERM
C
   30 XNORM = RMAX*DSQRT(SUM)
   99 RETURN
      END
```

SAMPLE INPUT

```
 4.00
 1
 4.20
 0
32
 1
 0.        1.000
 0.050     1.000
 0.083     1.000
 0.250     1.000
 0.500     1.000
 0.750     1.000
 1.080     1.000
 1.250     1.000
 1.500     1.000
 1.750     1.000
 2.000     0.961
 2.250     0.795
 2.750     0.690
 3.000     0.567
 3.083     0.462
 3.250     0.349
 3.667     0.292
 4.000     0.227
 4.250     0.187
 4.500     0.151
 4.750     0.128
 5.000     0.122
 5.250     0.129
 5.500     0.093
 5.750     0.093
 6.000     0.063
 6.250     0.075
 6.500     0.087
 7.800     0.046
 8.583     0.028
10.633     0.025
20.700     0.020
```

```
**********SAMPLE OUTPUT**********

O          INJECTION TIME

   4.0000808000088
O          NUMBER OF NONLINEAR PARAMETERS

  1
O          INITIAL ESTIMATES OF NONLIN. PARAM.

  4.200
O          NUMBER OF LINEAR PARAMETERS

  O
O          NUMBER OF OBSERVATIONS

 32
O          NUMBER OF INDEPENDENT VARIABLES

  1
O          INDEPENDENT VARIABLES

ØTIME vs MEASURED CONCENTRATIONS

  O.              1.000
  0.050           1.000
  8.883           1.000
  0.258           1.000
  8.500           1.000
  0.750           1.000
  1.000           1.000
  1.258           1.000
  1.500           1.000
  1.750           1.000
  2.800           6.961
  2.250           8.795
  2.750           8.690
  3.ØØØ           8.567
  3.883           8.462
  3.250           8.349
  3.667           8.292
  4.000           8.227
  4.250           8.187
  4.500           6.151
  4.750           8.128
  5.000           0.122
  5.250           8.129
  5.500           8.093
  5.750           0.093
  6.000           8.063
  6.250           8.075
  6.500           8.087
  7.800           8.046
  8.583           8.028
 10.633           8.025
 20.700           8.020
ØINCIDENCE MATRIX INC(1,1)=

  1
```

```
O    O  NORM OF RESIDUAL =  Ø.9Ø59386e+ØØ
      NU =  Ø.1ØØØØØØe+Ø1
O  ITERATION   1     NONLINEAR PARAMETERS
O  Ø.2916745e+Ø1
O     1  NORM OF RESIDUAL =  Ø.8Ø17488e+ØØ
      NU =  Ø.5ØØØØØØe+ØØ
      NORM(DELTA-ALF) / NORM(ALF) =   Ø.44Øe+ØØ
O  ITERATION   2     NONLINEAR PARAMETERS
O  Ø.24746Ø9e+Ø1
O     1  NORM OF RESIDUAL =  Ø.7871255e+ØØ
      NU =  Ø.25ØØØØØe+ØØ
      NORM(DELTA-ALF) / NORM(ALF) =   Ø.179e+ØØ
O  ITERATION   3     NONLINEAR PARAMETERS
O  Ø.245411Øe+Ø1
O     1  NORM OF RESIDUAL =  Ø.787Ø9Ø9e+ØØ
      NU =  Ø.125ØØØØe+ØØ
      NORM(DELTA-ALF) / NORM(ALF) =   Ø.835e-Ø2
O  ITERATION   4     NONLINEAR PARAMETERS
O  Ø.245437Øe+Ø1
O     1  NORM OF RESIDUAL =  Ø.787Ø9Ø9e+ØØ
      NU =  Ø.625ØØØØe-Ø1
      NORM(DELTA-ALF) / NORM(ALF) =   Ø.1Ø6e-Ø3
O  ITERATION   5     NONLINEAR PARAMETERS
O  Ø.2454356e+Ø1
O     1  NORM OF RESIDUAL =  Ø.787Ø9Ø9e+ØØ
      NU =  Ø.3125ØØØe-Ø1
      NORM(DELTA-ALF) / NORM(ALF) =   Ø.568e-Ø5
O  ITERATION   6     NONLINEAR PARAMETERS
O  Ø.2454357e+Ø1
O     1  NORM OF RESIDUAL =  Ø.787Ø9Ø9e+ØØ
      NU =  Ø.15625ØØe-Ø1
      NORM(DELTA-ALF) / NORM(ALF) =   Ø.373e-Ø6
O'''''''''''''''''''''''''''''''''''''''''''''''''''
O  NONLINEAR PARAMETERS

   Ø.2454357e+Ø1
Ø  NORM OF RESIDUAL =  Ø.787Ø9Ø9e+ØØ EXPECTED ERROR OF OBSERVATIONS = -Ø.7967799e-Ø1
   ESTIMATED VARIANCE OF OBSERVATIONS =  Ø.1998426e-Ø1
  WARNING -- EXPECTED ERROR OF OBSERVATIONS IS NOT ZERO.  COVARIANCE MATRIX MAY BE MEANINGLES

Ø'''''''''''''''''''''''''''''''''''''''''''''''''''
```

ØTIME VS CALCULATED CONCENTRATION

0.	1.000
0.050	1.000
0.083	1.000
0.250	8.999
0.580	17.998
0.750	17.995
1.ØØØ	8.990
1.250	17.981
1.500	8.968
1.750	8.948
2.ØØØ	Ø.922
2.250	8.888
2.750	0.798
3.000	8.744
3.083	8.725
3.250	8.686
3.667	Ø.583
4.000	8.500
4.250	8.440
4.500	8.383
4.750	8.330
5.000	8.281
5.250	8.238
5.500	8.199
5.750	8.165
6.000	8.136
6.250	Ø.111
6.500	8.090
7.800	8.027
8.583	8.012
10.633	8.001
20.700	8.ØØØ