FOREIGN TRAVEL REPORT

BELGIUM AND WEST GERMANY

MARCH 29 TO APRIL 13, 1986

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INTRODUCTION

This trip report discusses travel to two locations in foreign countries. The principal location visited was Ghent, Belgium, where I presented a paper entitled "An Evaluation of Constitutive Models for Salt Creep" at the 2nd International Symposium on Numerical Models in Geomechanics. Information related to this conference is attached. This segment was charged directly to our contract with the Office of Nuclear Waste Isolation (ONWI).

While attending the 5-day conference in Ghent, Belgium, I was invited to visit the facilities of the Federal Institute for Geosciences and Natural Resources (BGR) in Hannover, West Germany. I spent one day touring their new core storage and rock testing laboratory facility and discussing information related to my presentation in Ghent, Belgium. My host at the BGR was Manfred Wallner. This segment was not charged directly to ONWI.

ITINERARY

March 29	Travel from Rapid City, South Dakota to Washington, DC
March 30	Travel from Washington, DC to Ghent, Belgium
March 31 to April 4	Attend the 2nd International Symposium on Numerical Models in Geomechanics
April 5-6	Weekend
April 7	Vacation
April 8	Travel from Ghent, Belgium to Hannover, West Germany
April 9	Visit the Federal Institute for Geosciences and National Resources (BGR) and travel to Brussels, Belgium
April 10	Travel from Brussels, Belgium to Washington, DC
April 11	Vacation
April 12	Weekend
April 13	Travel from Washington, DC to Rapid City, South Dakota

PURPOSE OF TRIP

The primary purpose of this trip was to attend the 2nd International Symposium on Numerical Models in Geomechanics at Ghent, Belgium, and to present a paper entitled "An Evaluation of Constitutive Models for Salt Creep." A secondary purpose of the trip was to visit Professor J. P. Ottoy from the Applied Mathematics Department of the University of Ghent to discuss his computer program for a nonlinear curve-fitting technique. Also, I was invited to the BGR in Hannover, West Germany, to visit their facilities and to discuss the work that I presented at the symposium in Ghent.

ESSENTIAL DETAILS OF THE FOREIGN TRAVEL

March 31-April 3: I had discussions with Dr. Pande who was the co-chairman of the organizing committee of the symposium in Ghent, Belgium. I asked him why the vast majority of papers at this conference were related to soil mechanics. He thought that the distribution of papers between soil mechanics and rock mechanics reflected the geotechnical problems that currently exist. Also, he was reluctant to expand this conference beyond 100 presentations. We also discussed a prior request by Dr. Pande to publish an extended version of the paper that I submitted to this symposium. He is the editor of an international journal, Computers and Geotechnics, and hopes to release a special edition at the beginning of the next calendar year. I told him that it may be difficult because of the complications with the current study and the need for approval by ONWI and DOE.

April 2: I presented my paper entitled "An Evaluation of Constitutive Models in Geomechanics" at the 2nd International Symposium on Numerical Models in Geomechanics in Ghent, Belgium (see Attachment No. 1 and 2). As is usual at symposiums, there is not much time allocated for questions following the oral presentations of the paper. The questions that were asked were mainly related to clarification of the subject matter. Because my topic was unique and relevant to the theme of the symposium, I believe it was a worthy contribution to this symposium.

Several keynote lectures were given at this symposium, but the most interesting speech was given by Professor O. C. Zienkiewicz. Although his topic was related to soils, it was general enough to apply to the study of rock behavior. His main theme was to establish standardized tests for verification of models used in the soil mechanics community. Apparently, the issue of model verification is as important in soil mechanics as it is in rock mechanics. He admits that the various tests considered may not be applicable to all models, but that enough tests could be applied to any model to sufficiently evaluate its capability. Similarly, a standardization of tests to evaluate models in the rock mechanics community could be undertaken. Currently, models developed to characterize rock behavior are subjected to some types of verification problems, but all models are not verified in the same manner.

Although many of the papers presented at the conference were related to the mechanical behavior of soils, there were a few papers that directly related to the type of studies of rock behavior preferred at RE/SPEC Inc. In particular, a paper entitled "Thermal Structural Modeling of a Large Scale In-Situ Overtest Experiment for Defense High Level Waste at the Waste Isolation Pilot Plant Facility," by H. S. Morgan, C. M. Stone, R. D. Krieg, and D. E. Munson was presented at this conference. This paper dealt with the comparison of field measurements and numerical calculations that are related to some of the tests conducted at the Waste Isolation Pilot Plant (WIPP) near Carlsbad, New Mexico. Most of the comparisons of thermal behavior are good, whereas the comparisons of the displacements indicate that the field measurements can be as much as three times greater than the numerical calculations. Various sensitivity studies were performed to understand this substantial discrepancy. Their conclusions are that closure calculations may need to include some additional mechanical behavior such as damage, fracture, or plastic behavior. Also, the field measurements include the early-time displacements that are sometimes neglected by other investigators which tend to influence the closeness of comparisons between the measured and calculated displacements.

April 3: I met with Professor J. P. Ottoy who is at the University of Ghent in the Applied Mathematics Department in Ghent, Belgium. Professor Ottoy is a co-author of the paper entitled "A Computer Program for Non-Linear Curve Fitting," which was used in the study that I presented at the symposium in Ghent, Belgium. Because of this coincidence, I decided to set up a meeting between the two of us. He has not done much work on non-linear curve fitting since he published the paper. He did not credit himself with the derivation of the concepts presented in the paper, but rather he assembled the existing knowledge on related non-linear curve fitting techniques into a computer program. When I asked about the usage of the same shrinkage factors in the ridge regression, he thought that it would be advantageous to have unique shrinkage factors for each non-linear parameter of the expression. His response was interesting because we are currently using commercial software for non-linear regression (BMDP) that does provide individual shrinkage factors for ridge regression. He said he was motivated to create his own non-linear curve fitting program because of the difficulty in adapting commercial software, such as BMDP and SAS, to his needs.

I also asked his opinion on the tradeoffs of fitting each laboratory test individually or combining all the tests and solving directly for a single set of parameters. Basically, he was not prepared to provide a response since he had never encountered a similar problem. He was interested in our expansion of his program to include multiple independent variables. Finally, he mentioned that several of the references in his paper are good sources for information related to non-linear regression. For example, papers entitled "An Algorithm for Least Squares Estimations of Non-Linear Parameters" by D. W Marquardt and "Iterative Methods for Solving Non-Linear Least Squares Problems" by V. Lereyra are good references. Professor Ottoy's paper is provided in Attachment No. 3.

April 8-9: I met with personnel of the BGR in Hanover, West Germany. I was given a tour of BGR's new core storage and rock testing laboratory. Among the items of interest was a display of several types of salt that exist at their proposed nuclear waste repository site. The existence of several types of salt further complicates their ability to characterize the thermomechanical behavior of the host rock. Many of their rock testing machines are relatively new. Among them are the 100-mm-diameter triaxial creep testing machine that is capable of applying a stress difference of 250 MPa and temperatures of 400°C. Another testing machine has been modified to study the effects of moisture on the creep response of salt. This effect appears to be significant and it will be documented in a report they plan to release in the near future. Also, they have developed a new measurement technique in which they can detect axial strains to the nearest micron.

Following the tour of the core storage and testing facilities, a meeting was held with Professor Langer, Dr. Wallner, Dr. Wipp, Dr. Shultz, and Dr. Albrecht of the BGR who are directly involved with the rock mechanic studies related to the German waste disposal program. Professor Langer is the head of this group. Also, Dr. Morgan of Sandia National Laboratories was in attendance. I presented information related to the paper I had written for the symposium in Ghent, Belgium. Following my presentation, discussion of model fitting continued with a series of questions and answers. Most of the questions were related to clarification of the approach to evaluate various models for salt creep. In general, they thought this attempt to evaluate models was unique and worthwhile, but since they have not attempted a similar study, they were not prepared to offer advice or suggestions based on their experiences.

ATTACHMENT NO. 1

AN EVALUATION OF CONSTITUTIVE MODELS FOR SALT CREEP

by

Ralph A. Wagner
Paul E. Senseny

ABSTRACT

Seven constitutive models are evaluated for their ability to calculate creep of salt. The parameter values for each model were determined from a nonlinear curve-fitting technique that considers 47 creep tests. The effective stresses and temperature conditions for these creep tests ranged from 3.5 to 31.1 MPa and 25°C to 200°C, respectively. The evaluation of the constitutive relations is based primarily on the difference between the measured and calculated strains. Also considered in the evaluation was the agreement between measured and predicted strain rates at the end of each creep test. An extension to the evaluation included a numerical simulation of an in situ experiment, which involves a spatially inhomogeneous stress state, with one of the more favorable constitutive models.

1 INTRODUCTION

Many structural problems involve materials that exhibit inelastic behavior when subjected to thermomechanical loads. The accurate prediction of this inelastic behavior using numerical methods requires the implementation of sophisticated constitutive models. Several constitutive models have been developed that attempt to characterize the inelastic response of a material. Because engineering problems that involve inelastic behavior can be so varied in terms of material type and loading conditions, it is difficult to choose which constitutive model will be the most appropriate for a particular application. In this study, seven constitutive models are evaluated for their ability to calculate creep of salt.

The parameter values for each constitutive model are determined from a nonlinear curve-fitting technique using a common data base consisting of 47 creep tests. The evaluation of the models is based on the ability to reproduce the behavior of the 47 creep tests. This quantitative evaluation contrasts other attempts to evaluate constitutive models which usually consider the forms of the models in terms of the micromechanisms or internal state variables that are supposed to characterize the inelastic behavior of the material.

2 METHODOLOGY

The objective of this study was to evaluate constitutive models with regard to their ability to predict the creep behavior of salt when subjected to a specified range of thermomechanical loading. To evaluate the constitutive models, their respective parameter values were determined by using a nonlinear curve-fitting technique [Ottoy and Vansteenkiste, 1983]. This minimization technique consists of concepts developed by Marquardt [1963] which are modified with an eigenvalue analysis to increase the computational efficiency. Also, included in this technique is a method developed by Golub and Pereyra [1973] in which only nonlinear parameters are required. Therefore, this nonlinear curve-fitting technique is based on proven and accepted concepts that should insure that appropriate parameter values are determined for each of the models.

The parameter values for each constitutive model were determined by minimization of the following expression:

$$\frac{\sum_{i=1}^{N} W_i \int_T \int_\sigma \int_t \left\{1 - \frac{\epsilon_c}{\epsilon_m}\right\}^2 dt\,d\sigma\,dT}{\int_T \int_\sigma \int_t dt\,d\sigma\,dT},$$

where:

N = Number of creep tests.

W_i = Weight factor to normalize the influence of data points in each creep test.

$\int_j$ = Integration over the domain of j (e.g., temperature, effective stress, and time).

ϵ_c = Calculated strain.

ϵ_m = Measured strain.

The data base of laboratory-measured strains was identical for each constitutive model. The iterative technique mentioned above is well suited to evaluate parameters that comprise highly nonlinear expressions, such as the constitutive models considered in this study. In most cases, the iterative procedure was terminated when the relative change in the sum-of-the-square error was less than 0.001 of a percent. Another attempt to standardize the determination of the parameter values was to integrate numerically the rate forms in the constitutive models in a similar manner.

Upon the determination of the parameter values, an evaluation of the constitutive models is possible with respect to their ability to reproduce the laboratory tests from which the values of their respective parameters were determined. The integrated error over the duration of each test between the measured and predicted strains is the primary criterion for ranking the constitutive models. Also, consideration is given for the relative difference of the measured and predicted strain rates at the end of each test.

Once the constitutive models were evaluated with respect to their ability to reproduce the creep tests, one of the more favorable models was used to predict the inelastic response of an in situ experiment. Fundamentally, this in situ test differs from the laboratory tests in that the time duration is longer, test specimen is larger, and the stress state is spatially inhomogeneous.

2.1 Data Bases

This study incorporates two distinct data bases which consist of laboratory and in situ measurements. The laboratory-measured strain data comprises an extensive data base that includes 47 triaxial creep tests of 100 mm diameter salt specimens from Avery Island, Louisiana. For computational efficiency, every other measured strain value was used in the determination of parameter values, but this still provided a data base that consisted of more than 25,000 data points, which is an average of more than 500 data points per test.

The matrix of effective stresses and temperatures in the creep tests includes a range from 3.5 to 31.1 MPa and 25°C to 200°C, respectively (Figure 1). Depending on the loading condition, the duration of each test varied between 1 and 200 days which represents nearly 2,000 total days of testing.

A series of corejack tests were performed to provide an in situ data base from test situations that can be readily modeled using numerical methods. The corejack test can be represented as an axisymmetric configuration with a uniform pressure boundary. One of the primary advantages of this type of in situ experiment is that the preexisting stress state in the surrounding salt is not a factor.

In the corejack test, the primary measurement is the temporal change in the diameter of a borehole that has an initial nominal diameter of 200 mm. This borehole is concentrically located within a cylinder of salt that is one meter in diameter and depth. Pressure is applied to the outer circumference of the hollow cylinder, but no axial loading or axial displacement constraint is applied. The temperature is maintained at either ambient or elevated to a prescribed level.

Eight in situ tests were performed with unique temperatures and stress conditions. Since it is not the intent of this study to perform a complete simulation of the in situ tests, only a representative corejack test (10 MPa and 60°C) was considered. This simulation provided an opportunity to evaluate the ability of one of the best fitting constitutive models to predict a test more complex than a creep test.

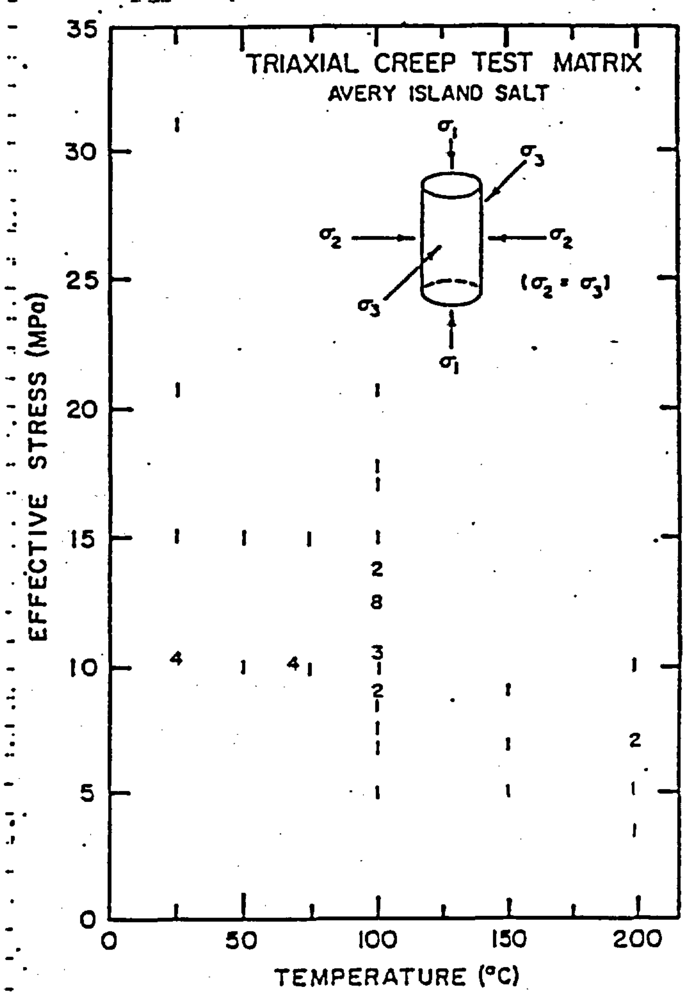

Fig. 1. Matrix of the 47 Creep Tests.

2.2 Constitutive Models

Seven constitutive models that are consistent with the phenomenalogy and micromechanics of salt have been selected from the literature. Although these seven constitutive models are representative of existing models, a continuation of this study is likely to incorporate additional models. For simplicity, only scalar (one-dimensional) forms that are compatible with triaxial compression are presented. Some of the models were developed to incorporate both loading and unloading, but only the loading portion was considered because the parameter values were determined from creep tests. In the model equations, σ is the effective stress, T is the absolute temperature, R is the universal gas constant, μ is the shear modulus, H is the heaviside function, ϵ is the inelastic strain, and $\dot{\epsilon}$ is the inelastic strain rate. If practical, the strain-rate forms of the models were integrated prior to the determination of the values of the fitting parameters. Consequently, the seven viscoplastic models are presented in either their strain or strain-rate form, depending on which form was used in the curve-fitting technique.

2.2.1 Munson-Dawson (M-D)

This model is based on the deformation mechanisms that are believed to control steady-state deformation over the ranges of stress and temperature that were imposed in the creep tests [Munson and Dawson, 1982]. The model emphasizes steady-state deformation; whereas, transient deformation is modeled empirically using the concept that the approach to steady state will be different depending upon whether the microstructure is hardening or softening (recovery). The micromechanisms that are incorporated in this model are dislocation glide, dislocation climb, and an undefined mechanism.

The equations that define this model are:

$$\begin{aligned} \epsilon &= \Theta\epsilon_t^*\left(1 - H\left(\epsilon - \epsilon_t^*\right)\right) \\ &\quad + \left(\epsilon_t^* + \dot{\epsilon}_{ss}t + \frac{\epsilon_t}{\Delta}\left(\exp^{-\Delta} - 1\right)\right) H\left(\epsilon - \epsilon_t^*\right), \end{aligned} \tag{1}$$

$$\Theta = 1 + \frac{1}{\Delta}\ln\left(\frac{\Delta}{\epsilon_t^*}\dot{\epsilon}_{ss}t + \exp^{-\Delta}\right) \tag{2}$$

$$\epsilon_t^* = K\left(\frac{\sigma}{\mu}\right)^m, \tag{3}$$

$$\Delta = \alpha + \beta\log\left(\frac{\sigma}{\mu}\right), \tag{4}$$

$$\dot{\epsilon}_s = \sum_{i=1}^{3}\dot{\epsilon}_{s_i}, \tag{5}$$

$$\dot{\epsilon}_{s_1} = A_1\exp^{-Q_1/RT}\left(\frac{\sigma}{\mu}\right)^{n_1} \quad \text{(dislocation climb)}, \tag{6}$$

$$\dot{\epsilon}_{s_2} = A_2\exp^{-Q_2/RT}\left(\frac{\sigma}{\mu}\right)^{n_2} \quad \text{(undefined mechanism)}, \tag{7}$$

and

$$\begin{aligned} \dot{\epsilon}_{s_3} &= 2\left(B_1\exp^{-Q_1/RT} + B_2\exp^{-Q_2/RT}\right) \\ &\quad \times \sinh\left[q\left(\frac{\sigma - \sigma_0}{\mu}\right)\right] H\left(\sigma - \sigma_0\right) \\ &\quad \text{(glide)}. \end{aligned} \tag{8}$$

There are 14 fitting parameters in this model: $A_1, A_2, B_1, B_2, K, m, \alpha, \beta, q, Q_1, Q_2, n_1, n_2$, and σ_0. The value of μ was assumed to be 9,620 MPa.

2.2.2 Ashby-Frost (A-F)

This model is also based on the micromechanisms that operate at steady state [Frost and Ashby, 1982]. However, no transient model is proposed by these authors. For simplicity, the Munson-Dawson transient model is adopted. The difference between the Ashby-Frost and Munson-Dawson models is the number and kind of mechanisms that are assumed to operate and the functional form appropriate for each mechanism.

The equations that define this model are:

$$\begin{aligned} \epsilon &= \Theta\epsilon_t^*\left(1 - H\left(\epsilon - \epsilon_t^*\right)\right) \\ &\quad + \left(\epsilon_t^* + \dot{\epsilon}_{ss}t + \frac{\epsilon_t}{\Delta}\left(\exp^{-\Delta} - 1\right)\right) H\left(\epsilon - \epsilon_t^*\right), \end{aligned} \tag{9}$$

$$\Theta = 1 + \frac{1}{\Delta}\ln\left(\frac{\Delta}{\epsilon_t^*}\dot{\epsilon}_{ss}t + \exp^{-\Delta}\right) \tag{10}$$

$$\epsilon_t^* = K\left(\frac{\sigma}{\mu}\right)^m, \tag{11}$$

$$\Delta = \alpha + \beta\ln\left(\frac{\sigma}{\mu}\right), \tag{12}$$

$$\dot{\epsilon}_s = \sum_{i=1}^{4}\dot{\epsilon}_{s_i}, \tag{13}$$

$$\dot{\epsilon}_{s_1} = A_1\left(\frac{\sigma}{\mu}\right)^2\exp\left[-\frac{\Delta F}{RT}\left(1 - \frac{\sigma}{\hat{\tau}}\right)\right] \quad \text{(glide)}, \tag{14}$$

$$\begin{aligned} \dot{\epsilon}_{s_2} &= \frac{A_2\mu}{T}\left(\frac{\sigma}{\mu}\right)^n\left\{\exp\left[-\frac{Q_v}{RT}\right]\right. \\ &\quad \left. + A_2'\left(\frac{\sigma}{\mu}\right)^2\exp\left[-\frac{Q_c}{RT}\right]\right\} \\ &\quad \text{(climb)}, \end{aligned} \tag{15}$$

$$\dot{\epsilon}_{s_3} = A_3\frac{\mu}{T}\left(\frac{\sigma}{\mu}\right)\exp\left[-\frac{Q_v}{RT}\right] \quad \text{(Harper – Dorn creep)}, \tag{16}$$

$$\dot{\epsilon}_{s_4} = A_4 \left(\frac{\sigma}{\mu}\right) \frac{\mu}{Td^2} \left(\exp\left[-\frac{Q_v}{RT}\right] + \frac{A'_4}{d} \exp\left[-\frac{Q_b}{RT}\right]\right) \quad (17)$$

(diffusional flow).

There are 16 fitting parameters in this model: A_1, ΔF, τ, A_2, n, A'_2, A_3, A_4, A'_4, K, m, α, β, Q_v, Q_b, and Q_c. The average grain size, d, was taken to be 0.0075 m and the expression for μ is given below:

$$\mu = 11{,}000(1. + (300 - T) * 6.797 \times 10^{-4}) \text{ MPa}.$$

2.2.3 Krieg (KRG)

This model uses a single internal variable, α, to incorporate thermomechanical history [Krieg, 1982]. This variable has the dimensions of stress (MPa) and is referred to as the backstress. Micromechanically, the backstress can be related to the mobile dislocation density. Hardening (or softening), such as occurs during transient creep, results from an increase (or decrease) in the backstress, which corresponds to an increase (or decrease) in the mobile dislocation density. Steady state is reached when the hardening and softening balance and the backstress becomes constant.

The equations that define this model are:

$$\dot{\epsilon} = A \exp\left(q\left|\sigma - \alpha\right|\right)(\sigma - \alpha), \quad (18)$$

$$\dot{\alpha} = B\dot{\epsilon} \exp\left[-\varsigma\alpha \operatorname{sgn}(\sigma - \alpha)\right] - C\left|\alpha\right|\alpha, \quad (19)$$

where

$$\begin{aligned} A &= A_0 \exp\left(-Q_A/RT\right) \\ B &= B_0 \exp\left(+Q_B/RT\right) \\ C &= C_0 \exp\left(-Q_C/RT\right) \\ \operatorname{sgn}(\sigma - \alpha) &= \begin{cases} +1, \sigma \geq \alpha \\ -1, \sigma < \alpha \end{cases} \end{aligned}$$

There are 8 fitting parameters in this model: A_0, Q_A, B_0, Q_B, C_0, Q_C, q, and ς.

2.2.4 Exponential-Time (E-T)

This model is based on the assumption that creep strain rate is governed by first-order kinetics [Senseny, 1983]. The steady-state strain rate is controlled by a thermally-activated mechanism. A critical strain rate divides the relationship of transient and steady-state responses into two regimes.

The equations that define this model are:

$$\epsilon = \dot{\epsilon}_{ss}t + \epsilon_a\left[1 - \exp^{(-\varsigma t)}\right], \quad (20)$$

$$\dot{\epsilon}_{ss} = A\sigma^n \exp^{(-Q/RT)}, \quad (21)$$

$$e_a = \frac{\epsilon_a}{\dot{\epsilon}^*_{ss}}\dot{\epsilon}_{ss} - \frac{\epsilon_a}{\dot{\epsilon}^*_{ss}}\left(\dot{\epsilon}_{ss} - \dot{\epsilon}^*_{ss}\right) H\left(\dot{\epsilon}_{ss} - \dot{\epsilon}^*_{ss}\right), \quad (22)$$

$$\varsigma = B\dot{\epsilon}^*_{ss} + B\left(\dot{\epsilon}_{ss} - \dot{\epsilon}^*_{ss}\right) H\left(\dot{\epsilon}_{ss} - \dot{\epsilon}^*_{ss}\right), \quad (23)$$

There are 6 fitting parameters in this model: n, Q, A, B, ϵ_a, and $\dot{\epsilon}^*_{ss}$.

2.2.5 Endochronic (ENDO)

The endochronic model is based on the irreversible thermodynamics of internal variables. The theory assumes that the current stress is a function of the strain history with respect to a time scale that is not the absolute time scale measured by the clock, but a time scale which is a material property [Valanis, 1971]. A significant difference between the endochronic model and the other models discussed in this study is that the elastic deformation is an integral part of the model. Therefore, only the strain that results from thermal expansion needs to be added to the strain predicted by this model to obtain total strain.

The equation that defines this model is:

$$\dot{\epsilon} = \dot{\epsilon}_0 \exp\left[1. - \frac{E}{\sigma}\exp(Q/RT)\exp \times \left(\frac{\beta E}{\sigma}\exp(Q/RT)\epsilon\right)\right]. \quad (24)$$

There are 4 fitting parameters in this model: $\dot{\epsilon}_0$, E, Q, and β.

2.2.6 Texas A&M University (TAMU)

This model is based on the concept of an equation of state which uniquely relates the state variables. Internal variables which represent the microstructure are not incorporated explicitly in the model. The influence of the evolving substructure is, however, introduced through a hereditary integral that contains a fading memory of strain-rate history [Russell et al., 1985].

The equation that define this model is:

$$\dot{\epsilon} = \left[\frac{1}{r_3 K}\sigma \exp^{-B/T}\right]^{\frac{1}{\eta}} \quad (25)$$

$$\left[(1. - \exp^{-r_1\epsilon}) + C\left(1 - \exp^{-r_2\epsilon}\right)\right]^{\frac{-2.}{\eta}}$$

$$\left[r_3(1 + C) - (r_1 + r_3)\exp^{-r_1\epsilon} - C\left(r_2 + r_3\right)\exp^{-r_2\epsilon} + r_1 \exp^{-(r_1+r_3)\epsilon} + Cr_2 \exp^{-(r_2+r_3)\epsilon}\right]^{\frac{1}{\eta}}.$$

There are 7 fitting parameters in this model: K, q, B, r_1, r_2, r_3, and C.

2.2.7 Bodner-Partom (B-P)

This model is characterized by a single internal variable, Z, that represents the material resistance to plastic flow by dislocation motion and which can be interpretted as a measure of the stored energy of cold work [Stouffer and Bodner, 1982]. No temperature dependence has been proposed previously for this model. Because the equations are somewhat similar to those of Krieg, the temperature dependence is assumed to be similar to the temperature dependence assumed by Krieg.

The equations that define this model are:

$$\dot{\epsilon} = \frac{2}{\sqrt{3}} D \exp\left\{-\frac{1}{2}\left[\frac{Z}{\sigma}\right]^{2n}\left(\frac{n+1}{n}\right)\right\}, \qquad (26)$$

$$\dot{Z} = m\left[Z_1 - Z\right]\sigma\dot{\epsilon} - AZ_1\left(\frac{Z - Z_2}{Z_1}\right)^r, \qquad (27)$$

where

$$\begin{aligned} D &= D_0 \exp\left[-Q_D/RT\right] \\ m &= m_0 \exp\left[Q_m/RT\right] \\ A &= A_0 \exp\left[-Q_A/RT\right]. \end{aligned}$$

There are 10 fitting parameters in this model: r, n, Z_1, Z_2, D_0, m_0, A_0, Q_D, Q_m, and Q_A.

3 MODEL FITTING RESULTS

The values determined for each set of fitting parameters of the seven constitutive models are presented in Table 1. An examination of these parameter values indicates that some terms of the constitutive models will have a negligible influence on the calculated strains for loading conditions considered in this study.

Once the parameter values were established, the constitutive models were evaluated based on two criteria. The minimization of error between the measured and calculated strains was taken to be the most important criterion. Also, close agreement between the measured and calculated strain rates at the end of each creep test was considered. Both of these criteria will help to assess the ability of the models to predict responses beyond the duration of the creep tests.

Figures 2 through 4 show strain-versus-time curves corresponding to the seven constitutive models and the laboratory measurements. These types of graphs allow relative evaluation of the model's ability to fit the measured creep response. Since it was not practical to present all 47 creep tests, a cross section of the thermal and mechanical loading conditions in the 47 test matrix are provided in these figures. The respective temperature/effective stress conditions for the three tests are 25°C/15 MPa, 100°C/10 MPa, and 200°C/3.5 MPa. Although these three creep tests are representative of the 47 creep tests, it would be inappropriate to infer that the trends diagnosed in Figures 2 through 4 exist for all 47 creep tests.

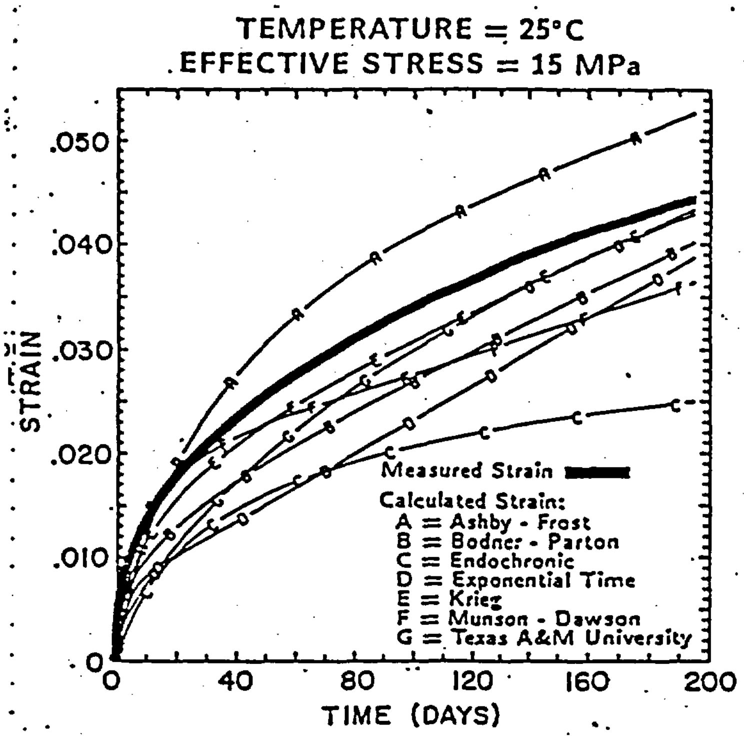

Fig. 2. Comparison of the Constitutive Models Ability to Simulate a Creep Test in Salt With a Temperature of 25°C and Effective Stress of 15 MPa.

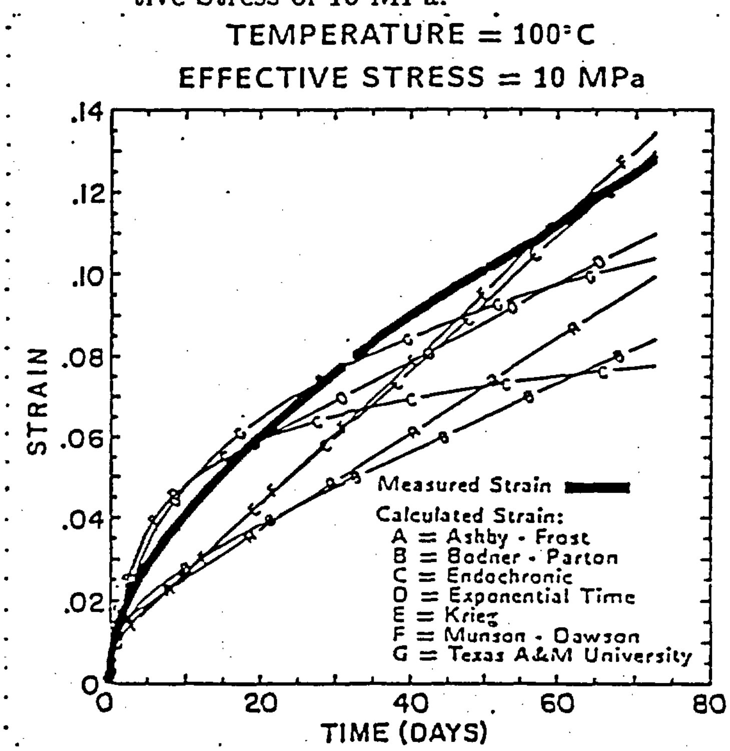

Fig. 3. Comparison of the Constitutive Models Ability to Simulate a Creep Test in Salt With a Temperature of 100°C and Effective Stress of 10 MPa.

Table 1. Parameter Values for the Constitutive Models Based on Avery Island Salt

Munson-Dawson[1]		Ashby-Frost[2]		Krieg		Endochronic		Bodner-Partom	
Parameters	Value	Parameters	Value	Parameters	Value	Parameter	Value	Paramter	Value
A_1 (sec^{-1})	4.87×10^{25}	A_1 (sec^{-1})	1.91×10^{5}	A_0	7.67×10^{-3} ($MPa^{-1} - sec^{-1}$)	$\dot{\epsilon}_0$ (sec^{-1})	7.84×10^{-6}	r	0.893
A_2 (sec^{-1})	2.12×10^{10}	ΔF (cal/mole)	1.32×10^{4}	Q_A	9632. (cal/mole)	E (MPa)	1.19	n	0.087
B_1 (sec^{-1})	1.47×10^{12}	r (MPa)	118.	B_0	168. (MPa)	Q (cal/mole)	2692.	Z_1 (MPa)	6.95×10^{5}
B_2 (sec^{-1})	0.978	A_2 (K/MPa - sec)	3.11×10^{8}	Q_D	2384. (cal/mole)	β	2.01	Z_2 (MPa)	3.12×10^{5}
K	1491.	n	23.9	C_0	0.400 ($MPa^{-1}-sec^{-1}$)	TAMU		D_0 (sec^{-1})	2.03×10^{18}
m	1.71	A'_2	9.87×10^{11}	Q_C	1.17×10^{4} (cal/mole)	K ($MPa - sec^q$)	3.11	m_0 (MPa^{-1})	2.11
α	-1.78×10^{-11}	A_3 (K/MPa - sec)	3.60×10^{-9}	q	0.232 (1./MPa)	q	0.158	A_0 (sec^{-1})	37.0
β	-1.46	A_4 ($K - m^2/MPa - sec$)	1.51×10^{-14}	ς	0.317 (1./MPa)	B (K)	1358.	Q_D (cal/mole)	1.30×10^{4}
q	3267.	A'_4 (m)	1.27×10^{-4}	Exponential-Time		r_1	625.	Q_m (cal/mole)	865.
Q_1 (cal/mole)	3.74×10^{4}	K	4.01×10^{5}	n	3.53	r_2	0.165	Q_A (cal/mole)	1.48×10^{4}
Q_2 (cal/mole)	1.38×10^{4}	m	2.42	Q (cal/mole)	9480.	r_3	1570.		
n_1	8.00	α	-10.46	A ($MPa^{-n} - sec^{-1}$)	1.22×10^{-6}	C	41.4		
n_2	3.35	β	-4.58	B	168.				
σ_0 (MPa)	9.20	Q_v (cal/mole)	1.13×10^{-8}	ϵ_a	0.078				
		Q_b (cal/mole)	5.29×10^{4}	$\dot{\epsilon}^*_{ss}$ (sec^{-1})	2.15×10^{-8}				
		Q_c (cal/mole)	2.36×10^{4}						

[1] Assumes $\mu = 9620$ MPa

[2] Assumes $\mu = 1.10 \times 10^4 \; (1. + (300 - T) * 6.79 \times 10^{-4})$ MPa

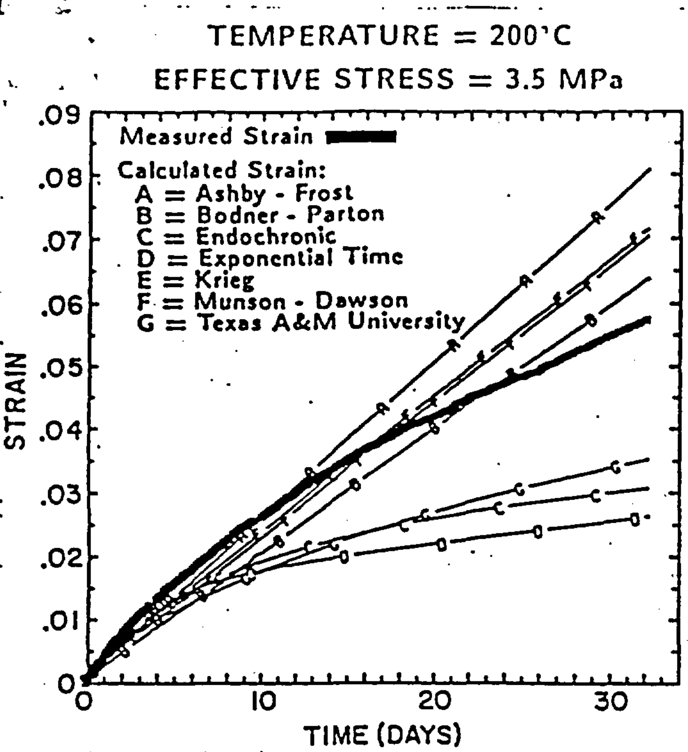

Fig. 4. Comparison of the Constitutive Models Ability to Simulate a Creep Test in Salt With a Temperature of 200°C and Effective Stress of 3.5 MPa.

The evaluation of the constitutive models abilities to reproduce all 47 creep tests can be assessed by determining the number of tests in which the relative difference in the measured and predicted strains is within a specified percentage. The bar chart shown in Figure 5 shows this type of comparison between the seven constitutive laws. Based on this criterion, the Munson-Dawson, Krieg, and Bodner-Partom models performed relatively well because the calculated strains were within 20 percent of the measured strains for more than one-half of the 47 creep tests. The remaining constitutive models appear to perform comparatively similar except for a slight improvement by the Ashby-Frost model in which the predicted strains were within 30 percent of the measured strains for approximately 70 percent of the creep tests.

The models ability to reproduce the measured strain rates at the end of the test is shown graphically in Figure 6. These bar charts indicate a close agreement between all of the models except for the endochronic models. This result is interesting because it identifies a different grouping of constitutive models than was evident when strain prediction was considered (Figure 5).

Based on the above results, it appears that the Munson-Dawson, Ashby-Frost, Krieg, and Bodner-Partom have performed relatively well in reproducing creep strains and strain rates that were measured in the 47 laboratory creep tests. The next grouping of constitutive models consists of the Texas A&M University, exponential-time, and endochronic models. The Texas A&M University and exponential-time models appear to predict the creep strain rates at the end of the test relatively well, but all three models had relative difficulty in predicting creep strains. This is disconcerting because the error between the measured and predicted strains was the basis for the minimization technique used to determine the fitting parameter values for each model.

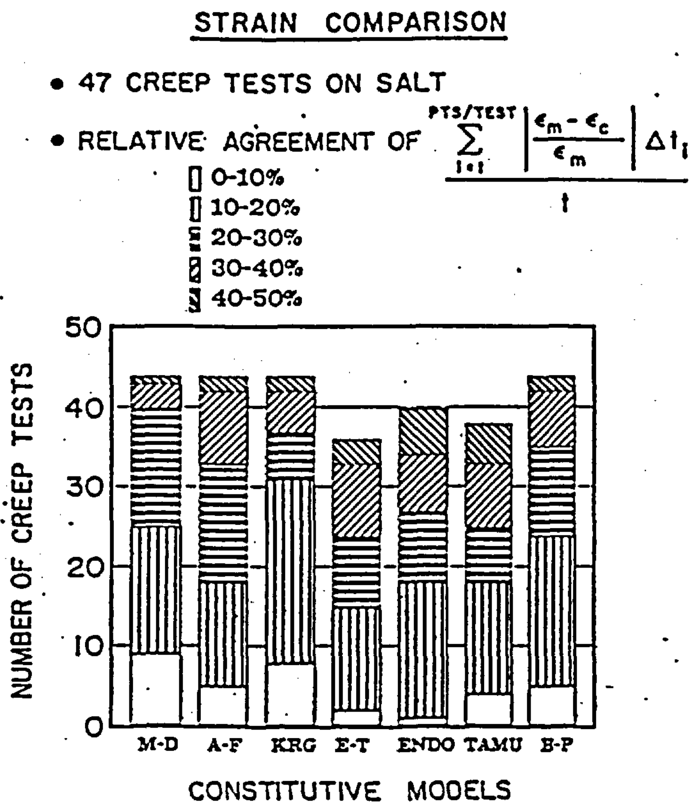

Fig. 5. Comparison of the Ability of the Constitutive Models to Simulate Laboratory-Measured Creep Strain.

4 PREDICTION OF AN IN SITU EXPERIMENT

An in situ experiment was designed in which the stress state is inhomogeneous, but the geometry and thermomechanical loading conditions could be accurately simulated by the finite element method. The Munson-Dawson model, which is one of the more favorable constitutive models, was used to simulate this test. Since the parameter value for unloading in the Munson-Dawson model could not be determined from the creep tests, a value was obtained from a study performed by Munson and Dawson [1982]. This approximation is adequate because a subsequent calculation was performed without the unloading parameter, and the difference in borehole closure was less than one-tenth of a percent. The loading conditions in the in situ experiment consisted of the radial pressure of approximately 10 MPa and a constant temperature distribution of 60°C.

The comparison of the predicted and measured borehole closure along the midheight of the corejack test is shown in Figure 7. The agreement between the measured and predicted borehole closure is encouraging. Although only one in situ experiment was considered, the results indicate an improvement over a recent simulation of this in situ experiment that was performed prior to this evaluation of constitutive models.

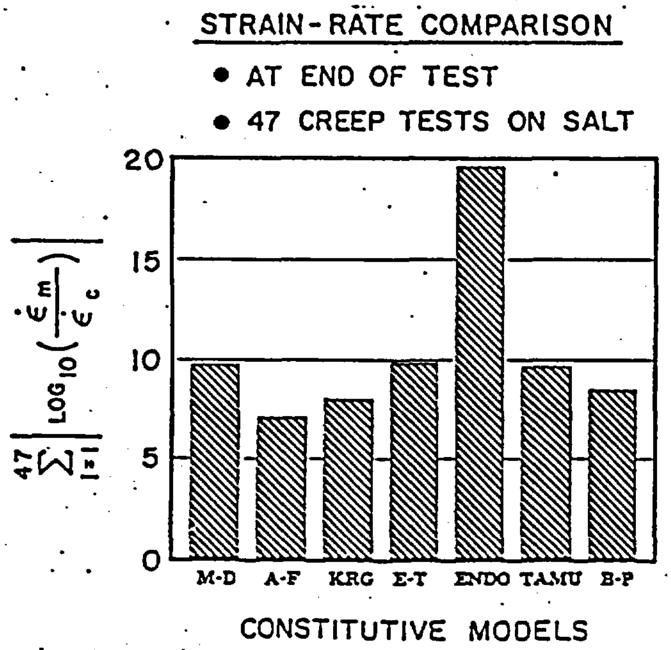

Fig. 6. Comparison of the Ability of the Constitutive Models to Simulate Laboratory-Measured Strain Rates at the End of the Creep Tests.

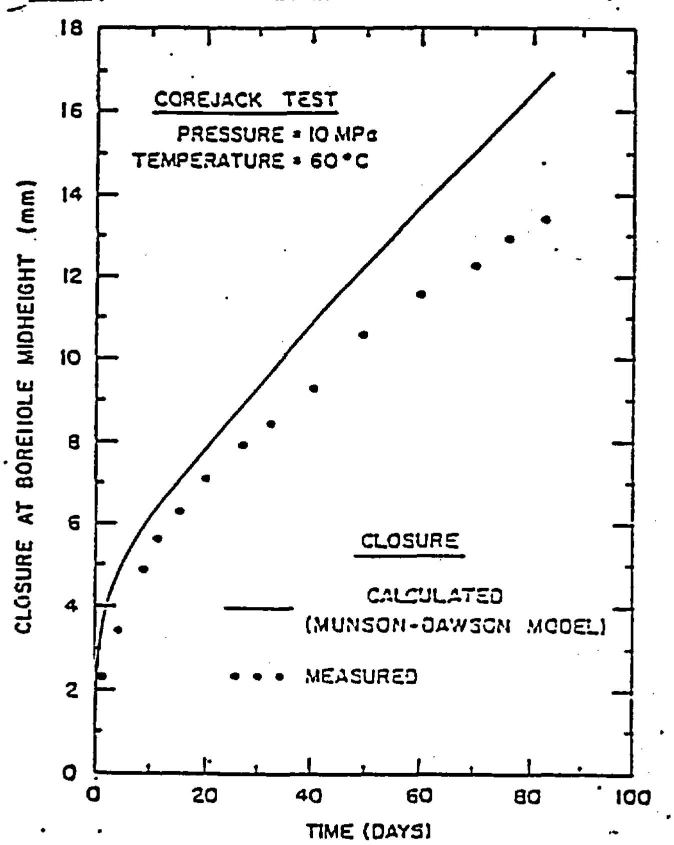

Fig. 7. Comparison of Calculated and Measured Deformations for In Situ Experiment.

5 CONCLUSIONS

This evaluation has provided insight to the adequacy of seven constitutive models to simulate the creep response of salt. For the conditions considered in this study, it appears that the seven constitutive laws can be grouped into two categories of performance. The Munson-Dawson, Ashby-Frost, Krieg, and Bodner-Partom models performed relatively well in reproducing the creep strains and strain rates that were measured in the 47 laboratory creep tests. The next grouping of models consists of the Texas A&M University, exponential-time, and endochronic models which perform comparatively similar in terms of reproducing the inelastic response of the creep tests.

This type of study cannot be performed without the evolution of other related substudies and/or improvements. Some important aspects not addressed in this study would include an investigation of the individual contribution of the micromechanisms or internal variables that comprise the formulation of some of the models. This may lead to a formulation of a more representative constitutive model that incorporates the favorable segments of various constitutive models. The data base of laboratory tests needs to be expanded to include tests with unloading so that the models that incorporate recovery can be evaluated more fully. An investigation of various nonlinear curve-fitting techniques need to be performed to find the most appropriate method for determining parameter values. The method used in this study [Ottoy and Vansteenkiste, 1983] is based on accepted concepts, but other nonlinear curve-fitting techniques may exist that are easier to apply and computationally more efficient. Other models need to be considered to insure that the most representative model is selected for the conditions considered. Finally, the brittle behavior of salt needs to be modeled to provide a more complete simulation of structural problems that exist in salt.

This study has presented a method to evaluate constitutive models. Although some adjustments could enhance this method, this study did identify the more appropriate models that should be considered for further evaluation.

ACKNOWLDEGEMENTS

This study was performed under a subcontract with Battelle Memorial Institute, a Department of Energy contractor. The subcontract was administered by the Office of Nuclear Waste Isolation. The authors are grateful for the opportunity to have performed this study in this contractual environment.

Technical assistance was provided by Dr. Joe L. Ratigan. Ms. Karen M. Linde is to be credited for the graphical representation of the results, and Ms. Cami D. Buller is responsible for the typing of the manuscript.

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ATTACHMENT NO. 2

INFORMATION RELATED TO THE
2nd INTERNATIONAL SYMPOSIUM ON
NUMERICAL MODELS IN GEOMECHANICS

2nd International Symposium

on

NUMERICAL MODELS IN GEOMECHANICS

(NUMOG II)

under the Royal patronage of His Majesty the King Boudewijn

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Host

Labratorium voor Grondmechanica
State University of Ghent
Belgium

31 March - 4 April, 1986
Ghent State University
Ghent
BELGIUM

CONFERENCE ARRANGEMENTS

HOW TO REACH GHENT

There are Sabena Airlines coaches from Brussels airport to Ghent - St-Pieters at 7.30, 10.30, 13.30, 16.30, and 19.00 hours. Journey time is one hour. If you arrive at a time when there is no convenient coach, take a train to Brussels Central and change for Ghent-St-Pieters. Journey time can vary from 50 to 90 minutes. You should buy a ticket for Ghent-St-Pieters. Price approximately B.Fr. 200

ACCOMMODATION

Take a taxi for Holiday Inn (if you have made a booking there) or to your down town hotel. See map for the location of Holiday Inn.

REGISTRATION

Delegates can register in the foyer of Holiday Inn from 18.00-21.00 hrs. on Sunday, 30 March. They can also register between 9.00-11.00 on Monday, 31 March in the foyer of the Congress Hall (see map) where all technical sessions will be held.

Those who arrive late can register during coffee breaks in the foyer of the Congress Hall.

TRANSPORT

Regular transport will be provided between Holiday Inn and the Congress Hall according to the timings of the technical and social programmes.

LECTURES

Keynote lectures by the invited speakers will be held in the main auditorium of the Congress Hall. Two sessions for presentation of papers will run in parallel in smaller lecture theatres.

PRESENTATION OF PAPERS

Time allocated for presentation of papers including discussion is normally twenty minutes. For each session the presenters of papers must see their Session Chairman beforehand. Two slide projectors and an overhead projector will be available. If you require any special facilities for your presentation, please let us know in advance.

EXHIBITION

A number of engineering companies and publishers of technical books will be setting up displays in the foyer of the Congress Hall where their representives will be available.

SOCIAL PROGRAMME

There is a full social programme for the delegates. The details are as follows:

Monday 31 March	Reception 19.30 - 22.300 hrs. at The Europa Hotel, Gordunaleaai, Ghent

Tuesday	1 April	Concert 20.30 hrs.
Wednesday	2 April	Boat trip - sight seeing
Thursday	3 April	Conference banquet in St. Pieters Abbey, 20.00 hrs.

LADIES PROGRAMME

An accompanying persons programme will be arranged. In addition to the participation of the social programme for the delegates as above, it will include a day trip to Brussels, a day trip to Brugge and a conducted tour of the city of Ghent and environs. Price B.fr. 7000. For further details write to: Mrs. Christiane Bonte, Fiesta Reizen N.V., Zuidstraat 21, B-8800 ROESELARE, Belgium. Tel.(051)222 288 before 1st. March 1986.

WEATHER

Weather in Ghent during April is variable. Please bring sufficient warm clothing and rain-wear.

PROCEEDINGS

Proceedings of the symposium will be availabe to all the delegates at the conference. Additional copies may be ordered from the publishers M. Jackson & Son (Publishers) Ltd., Station Hill, REDRUTH, Cornwall, TR15 2AX, England.

PROVISIONAL PROGRAMME

SUNDAY 30 MARCH

18.00 - 21.00 REGISTRATION IN HOLIDAY INN

MONDAY 31 MARCH

9.00 - 11.00 REGISTRATION IN CONGRESS HALL

11.00 - 11.45 WELCOME

12.00 - 14.00 LUNCH

14.00 - 14.35 KEYNOTE LECTURE: B. B. BROMS

Experience with finite element analysis of braced excavation in Singapore.

14.40 - 15.40 Session 1 A

The plastic equilibrium of a Coulomb-Rowe medium
P. De Simone

Interpretation of hardening-softening rule
E. Evgin & Z. Eisenstein

A mathematical description of elstoplastic deformation in normal yield and sub-yield states
K. Hashiguchi

14.40 - 15.40 Session 1 B

Comparison between centrifugal and numerical modelling of unsupported excavation in sand
R. Azevedo & H. Y. Ko

Comparision of numerical and experimental results for buried pipes
A. B. Fourie & G. Beer

Identification of parameters in tunnel excavation problem
A. Ledesma, A. Gens & E. E. Alonso

15.40 - 16.00 COFFEE BREAK

16.00 - 17.40 Session 1 A (continued)

Initial state for anisotropic elasto-plastic model
F. Molenkamp & A. van Ommen

An extention to the deformation theory of plasticity
P. A. Vermeer & G. J. M. Schotman

Soil structure directionally dependent interface constitutive equation - application to prediction of shaft friction along piles
M. Boulon & C. Plytas

A Pseudo-elastic stress constitutive operator for soils
A. G. Kasim & W. N. Houston

Flow surface model of viscoplasticity for normally consolidated clay
T. Matsui & N. Abe

16.00 - 17.40 Session 1 B (Continued)

Stability of soil and rock masses-factor of safety calculated by nonlinear analysis and by linear programing
A. C. Matos, P. S. Marques & J. B. Martins

Three dimensional simulation of rock-liner interaction near tunnel face
F. Pelli, P. K. Kaiser & N. R. Morgenstern

Numerical solutions for the axisymmetric tunnel problem using Hoek-Brown criterion
M. B. Reed

The influence of joint orientation and elastic anisotropy in analysis of tunnels in jointed rock masses
H. F. Schweiger, W. Aldrian & W. Haas

The elastic response of cylindrical rock anchors with base delaminations
A. P. S. Selvadurai & M. C. Au

).30 RECEPTION at The Europa Hotel, Gordunaleaai, Ghent, hosted by n. v. Pieux Franki

JESDAY 1 APRIL

00 - 9.35 KEYNOTE LECTURER: A. VERRUIJT

A finite element model for simultaneous flow of fresh and salt ground water

9.40 - 11.00 Session 2 A

Modelling of sand behaviour with bounding surface plasticity
J. Bardet

Numerical simulation of shear-band bifurcation in sand bodies
R. de Borst

A theoretical model using a few number of parameters
S. Chaffois & J. Monnet

A numerical model analysing free torsion pendulum results
O. Storrer, H. Van Den Broeck & W. F. Van Impe

9.40 - 11.00 Session 2 B

Finite element analysis of steel lined branching tunnels
D. V. Thareja, K. G. Sharma & K. Madhavan

Finite element analyses of retaining walls
K.J.Bakker & P. A. Vermeer

Lateral earth pressure development from at-rest to active behind retaining walls
S. Bang & H. T. Kim

Semi-analytical approach to no contact tension problems
I. D. Desai & V. S. Chandrasekaran

11.00 - 11.20 COFFEE BREAK

11.20 - 11.55 KEYNOTE LECTURE: W. D. L. FINN

12.00 - 13.00 Session 2 A (Continued)

A cyclic viscoplastic constitutive equation for soils with kinematic hardening
D. Aubry, Y. Meimon & E. Kodaissi

Shear band analysis in granular material by Cosserat theory
H. B. Muhlhaus

A constitutive model for anisotropic granular media
R. Nova

12.00 - 13.00 Session 2B (Continued)

Numerical analysis of anchored reinforced concrete diaphragm walls
R. Folic & P. Pavlovic

Three dimensional analysis of flexible earth retaining structures
H. Matoes Fernandes

Analysis of compaction induced stresses and deformations
R. B. Seed & J. H. Duncan

13.00 - 14.30 LUNCH BREAK

14.30 - 15.05 KEYNOTE LECTURE: J. GHABOUSSI

Two - dimensional and three - dimensional Discrete Element analysis

15.10 - 16.10 Session 3A

* A constitutive model for secondary consolidation
H. Akaishi, A. Tonosaki & G. N. Pande

A viscoplastic constitutive model of normally consolidated clay under three-dimensional stress condition
F. Oka

Modelling behaviour of stone column reinforced soft clays
H. F. Schweiger & G. N. Pande

15.10 - 16.10 Session 3B

Numerical analysis of soil-structure interaction problem in loess
S. M. Sargand & R. Janardhanam

Interaction between the bottom of cylindrical tank and soil
M. T. Heinisuo & K. A. Miethinen

* Interaction analysis of footing using an elstoplastic constitutive mode
R. Kuberan, K. G. Sharma & A. Vardarajan

16.10 - 16.30 COFFEE BREAK

16.30 - 17.50 Session 3A (Continued)

Three dimensional model for rock joints
I. Carol, A. Gens & E. E. Alonso

A constitutive model for jointed and fissured materials
S. Pietruszczak & D. F. E. Stolle

Anisotropic failure of a laminated sediment
P. Smart & B. M. A. Omer

Numerical model for jointed media
A. A. Serrano Gonzalez & A. Soriano

16.30 - 17.50 Session 3B (Continued)

Finite element analysis of dam foundations with seams
K. G. Sharma, A. Vardarajan & C. Chinnaswamy

A raft foundation on the London clay: A comparison between the predicted behaviour and the long term measurements
L. A. Wood & A. J. Perrin

Assessment of different excavation procedures in tunnel excavation
J. Xiang, J. Huai & J. Lu

Prediction of radial displacements at the face of shallow tunnels
A. Negro, Z. Eisenstein & H. Heinz

An examination of various constitutive relationship model with model pressuremeter test
G. Li & J. Pu

CONCERT 20.30

WEDNESDAY 2 APRIL

9.00 9.40 KEYNOTE LECTURE: O. C. ZIENKIEWICZ

* A general procedure for numerical solution of statics and dynamics of soils

9.45 - 10.45 Session 4A

Behaviour of Hostun sand under drained circular stress path
T. Doanh

O.C. Zienkiewicz.
" make things as simple as possible, but no simpler !"
. Standard tests should be established for verification of models. by the soil. mechanics community.

Uniaxial strain testing of soils in a split-Hopkinson pressure bar
C. W. Felice, E. S. Gaffney & J. A. Brown

The determination of appropriate soil stiffness parameters for use in finite element analyses of geotechnical problems
A. B. Fourie, D. M. Potts & R. J. Jardine

9.45 - 10.45 Session 4 B

Numerical modelling of pile driving
H. Balthaus & S. Kielbassa

Analysis of efficiencyof axially loaded pile groups
M. R. Madhav & B. B. Budkowska

The crack - expanded model and finite element analysis of creep of rock slope
Z. Tao & Q. Yu

Bearing capacity and displacements of column and pile foundation subjected to the horizontal forces
E. Dembicki & W. Odrobinski

10.45 - 11.00 COFFEE BREAK

11.00 - 12.00 Session 4 A (Continued)

A data acquisition and processing system for the triaxial test
E. Goelen, R. Carpentier & W. Verdonck

Comparison of models in deformation analysis of soft ground under embankment
Z. J. Shen & J. D. Yi

Evaluation of constitutive models for salt creep
R. A. Wagner & P. E. Senseny

11.00 - 12.00 Session 4 B (Continued)

Thermal structural modelling of alarge scal in-situ overtest experiment for defence high level waste at the waste isolation pilot plant facility
H. S. Morgan, C. M. Stone, R. D. Kreig & D. E. Munson

Calculating contaminant migration in groundwater using microcomputers
R. K. Rowe & J. R. Booker

Contact pressure and foundation forces with four soil models
Z. E. Yao & J. R. Zhang

12.00 - 1.30 LUNCH BREAK

13.30 - 17.30 SIGHT SEEING TOUR

THURSDAY 3 APRIL

9.00 - 9.35 KEYNOTE LECTURE: M. JAMEIOLKOWSKI

The role of experimental soil engineering in numerical models for geomechanics

9.40 - 10.40 Session 5 A

The behaviour of reinforced earth walls under self-weight and external loading
G. E Bauer & Y. M. Mowafy

A model to simulate excavations supported by nailing
A. S. Cardoso

FEM analyses of compacted reinforced soil walls
R. B. Seed, J. G. Collins & J. K. Mitchell

9.40 - 10.40 Session 5 B

The distinct element modelling for earthquake response analysis
T. Ohmachi & Y. Arai

The evaluation of wave fronts in a saturated porous medium
H. v. d. Kogel

Application of non linear surface wave response analysis to the liquefaction damage to Hachirogata reclaimed dyke due to Nihonkai Chabu Earthquake of 1983
S. Nakamura & E. Yanagisawa

10.40 - 11.00 COFFEE BREAK

11.00 - 13.00 Session 5 A (Continued)

Numerical modelling of reinforced embankment constructed on weak foundation
R. K. Rowe

Incremental analysis of layed viscoelastic half space
B. B. Budkowska

Study of soil geotextile interaction - a reinforced embankments
J. Honnet, J. P. Gourc & H. Hommessin

TRIADH: A constitutive model and its application to the prediction and analysis of embankment dam performance
Ph. Des. Croix & E. Frossard

Analysis of failure of an embankment on soft soil: A case study
J. A. H. Teunissen, Chr. H. H. Bauduin & E. O. F. Calle

Numerical prediction and real behaviour of a reinforcement system for a tunnel in Northern Italy
G. Barla & P. Jaree

11.00 - 13.00 Session 5 B (Continued)

Numerical modelling of non linearities in groundwater flow
J. A. H. Teunissen

Mathematical model for a controlled groundwaterlowering during the construction of the Berendrecht Sealock at Antwerp
H. Raedschelders, J. Maertens & S. Vanmarcke

Simulation of sand liquefaction in shaking table tests by two phase F.E. analysis
H. Hatanana et al

Dynamic behaviour of saturated sand: predictions based on multiple neutral loading loci concept
S. Pietruszczak & D. F. E. Stolle

Seismic response and liquefaction of embankments numerical solution and shaking table tests
T. Tanaka, H. Yasunaka & S. Tani

Finite element model to predict permanent displacement of ground induce by liquefaction
I. Towhata

Finite element analysis of coupled loading and consolidation
R. I. Woods

13.00 - 14.30 LUNCH BREAK

16.00 - 17.50 Session 6 A

Elastoplastic finite element analysis of undrained problems by a mixed weighted residual formulation
R. Correia

A transition element for consistent mesh refinement applied to creep analysis of rock sale
B. Kroplin, M. Schwesig, A. Honecker, H.K. Nipp & M. Wallner

A semi-analytical F.E. model for 3D soil foundation
J. Kujawski, N.E. Wiberg & M. Olejnik

Hybrid stress model in geomechanics
M. Sargand

Modelling of slope stability by the Boundary Element Method
H. Suchnicka & H. Konderla

Application of Distinct Element Method in geotechnical engineering
J.M. Ting, B. T. Corkum & C. Greco

Symmetric formulation of tangential stiffness for non-associated visco-plasticity
W. Xiong

1600 - 17.50 Session 6 B

Equivalent linear analysis in earth quake geotechnical engineering - a reappraisal
E. G. Prater

Boundary element solution for dynamic soil - structure interaction
O. Tullberg, Z. Xi-Reng & E. Wiberg

A numerical approach for the 3-D propagation and growth of hyddraulic fracture in a layered ground
S. B. Ammou

Analysis and design of hydraulic fracturing using a fully three dimensional simulator
K. Y. Lam

Variational solutions to boundary integral equations in elasticity and their application to three dimensional computation of fracture propagation
E. Touboul & K.B. Naceur

The experimental verification of two new numerical design methods for very heavy duty industrial pavements
J. W. Bull, M. H. H. M. Ismail & S. H. Salmo

14.30 - 15.05 KEYNOTE LECTURE: K. ISHIHARA

Influence of rotation of principal stress directions on the cyclic behaviour of sands

15.05 - 15.40 KEYNOTE LECTURE: A. N. SCHOFIELD

Advances in geotechnical centrifuge modelling

15.40 - 16.00 COFFEE BREAK

FRIDAY 4 APRIL

9.00 - 9. 35 KEYNOTE LECTURE: W. WITTKE

Finite element analyses and the stability of tunnels

9.35 - 10.10 KEYNOTE LECTURE: H. MEISSNER

10.10 - 10.40 Session 7

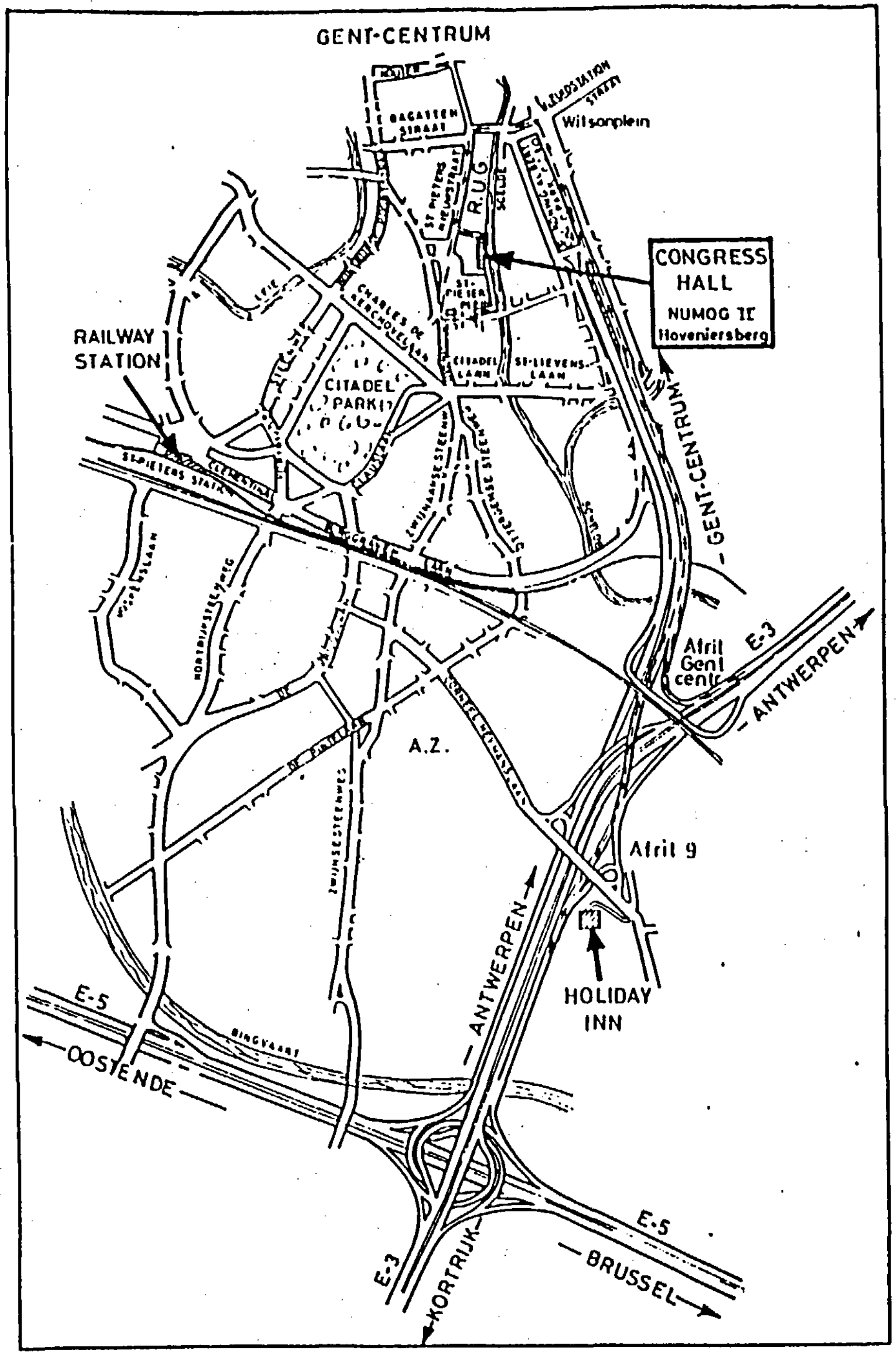
10.40 - 11.00 COFFEE BREAK

11.00 - 12.30 Panel discussion and closure

12.30 - 14.00 LUNCH

CONFERENCE PROGRAMME

	MONDAY 31/3	TUESDAY 1/4	WEDNESDAY 3/4	THURSDAY 3/4	FRIDAY 4/4
9 a.m. - 1 p.m.	9 a.m. - 11 a.m. REGISTRATION; 11 a.m. WELCOME	LECTURE 2 Prof. Verruijt; Technical Session 2A / 2B; COFFEE BREAK; LECTURE 3 Prof. Finn; Technical Session 2A / 2B	LECTURE 5 Prof. Zienkiewicz; Technical Session 4 A / 4 B; COFFEE BREAK; Technical Session 4A / 4B until 11.30 a.m.	LECTURE 6 Prof. Jamiolkowski; Technical Session 5A / 5B; COFFEE BREAK; Technical Session 5A / 5B	LECTURES 9 & Prof. Wittke, Prof. Meissner; Technical Session 7A / 7B; COFFEE BREAK; PANEL DISCUSSION & CLOSURE
2.30 p.m. - 5.30 p.m.	LECTURE 1 Prof. Broms; Technical Session 1A / 1B; COFFEE BREAK; Technical Session 1A / 1B	LECTURE 4 Prof. Ghaboussi; Technical Session 3A / 3B; COFFEE BREAK; Technical Session 3A / 3B	BOAT TRIP 1.30 p.m. - 6.30 p.m.	LECTURE 7 Prof. Ishihara; LECTURE 8 Prof. Schofield; COFFEE BREAK; Technical Session 6A / 6B	
	Reception	Concert Evening		Closing Banquet in St. Pieters Abbey	



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State University of Ghent, Ghent, Belgium
31st March - 4th April 1986

NUMOG II

Second International Conference on
NUMERICAL MODELS IN GEOMECHANICS

30 December 1985

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With season's greetings,

Yours sincerely,

Gyan Pandé

(G. N. PANDE)
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State University of Ghent, Ghent, Belgium
31st March - 4th April 1986

NUMOG II

Second International Conference on
NUMERICAL MODELS IN GEOMECHANICS

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PROF. Dr. ir. W.F. VAN IMPE,
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SYMPOSIUM THEMES

Numerical modelling of soil and rock behaviour under monotonic, cyclic and transient loading.

Numerical modelling of soil and rock reinforcements.

Comparison of numerical predictions with physical model tests and field measurements.

Applications of numerical models to the solution of practical geotechnical problems.

Microcomputers in geotechnical testing, analysis and design.

First Announcement
and Call for Papers

2nd International Symposium
on
NUMERICAL MODELS IN GEOMECHANICS

NUMOG II

31st March - 4th April 1986
GHENT STATE UNIVERSITY
BELGIUM

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Abstracts and enquiries regarding the conference should be addressed to : -

Dr. G.N. Pande,
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OBJECTIVES

The role of the finite element method in geotechnical engineering practice has been firmly established in recent years. The key to the successful solution of problems lies in the choice of appropriate numerical models and their associated parameters for geological media. Much research effort is currently in progress and a number of models are now available for application to practical problems.

The main objective of the symposium, second in the series - first was held at Zurich in 1982- is to provide a forum for discussion and exchange of views between researchers and practising engineers. A special emphasis will be given to the verification and evaluation of models for practical applications such as embankment dams, offshore structures, foundations, tunnels and underground structures, earth - retaining structures etc. Monotonic, cyclic and random loading including prediction of liquefaction potential under earthquake conditions will be discussed. Papers on verification of numerical models through physical model experiments are specially welcome.

CALL FOR PAPERS

Abstracts of papers, not exceeding 500 words, are invited on topics outlined overleaf.
These should be submitted before 31st July 1985. Final manuscripts will be due before 31st December 1985. All papers will be published in the proceedings of the symposium.

LOCATION

The symposium will be held at the State University of Ghent, Ghent, Belgium.

LANGUAGE

The official language will be English.

2nd International Syposium on
Numerical Models in Geomechanics
31st March - 4th April 1986
to be held at the
Ghent State University Ghent, Belgium.

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CONFERENCE FEES

The registration fees, inclusive of reception, lunches, conference proceedings and social programme are as follows :

	Before 31.12.85	After 31.12.85
Authors	£275	£300
Delegates	£300	£325
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ATTACHMENT NO. 3

A PROGRAM FOR A NONLINEAR CURVE-FITTING COMPUTER TECHNIQUE

by

J. P. Ottoy
G. C. Vansteenkiste

A computer program for non-linear curve fitting

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Recently several techniques for non-linear curve fitting have been developed. The implementation of a non-linear curve fitting procedure is treated for mathematical models in which the linear and the non-linear parameters are separable. The technique of Golub and Pereyra is used so that a minimization algorithm only for the non-linear parameters is needed. The minimization algorithm of Marquardt has been completed with an eigenvalue analysis. In order to reduce the computation steps the inverses of matrices of the form $A+\lambda I$ are calculated with the eigenvalues and eigenvectors of the matrix A. Of particular interest is the obtained convergence speed and the ease with which the method can be applied.

INTRODUCTION

During the last decade the techniques of non-linear curve fitting have emerged as an important subject for study and research. The increasingly widespread application of this subject has been stimulated by the availability of digital computers and the necessity of using them in complicated systems.

The intention of curve fitting can be: (a) to verify the correspondence between a mathematical model and some experimental data ($x_i, y_i, i=1, m$); (b) to determine certain unknown parameters by means of a valid supposed mathematical model. As long as all the parameters $a_i (i=1, n)$ are linear in the model, e.g. a model of the form:

$$y=a_0+a_1\varphi_1(x)+\ldots+a_n\varphi_n(x)$$

the determination of the unknown parameters is not difficult. They are solutions of the linear normal equations. However, if the model depends also on non-linear parameters, the fitting is more difficult and needs iterative methods. If there are several non-linear parameters, the computer time can therefore increase very rapidly. In this paper a computer program is described to fit in an efficient way a non-linear mathematical model. Only one independent variable x is considered, but the method can easily be extended for several independent variables.

It is supposed that the linear and the non-linear parameters are separable. A least squares problem is called separable if the fitting function can be written as a linear combination of functions $\varphi_j(\vec{b}; x)$ involving further parameters in a non-linear manner. Suppose the data (x_i, y_i, $i=1, m$) has to be fitted the model:

$$y=\varphi(\vec{a},\vec{b}; x)=\sum_{j=1}^{n} a_j\varphi_j(\vec{b}; x)+\varphi_0(\vec{b}; x) \tag{1}$$

with

$$\vec{a}\in R^n,\ \vec{b}\in R^k \text{ and } n+k\leqslant m$$

The functions $\varphi_j(\vec{b}; x)$ are not linear in $\vec{b}$. One has then to minimize the following sum of squares of deviations:

$$r_1(\vec{a},\vec{b})=\sum_{i=1}^{m}\left[y_i-\varphi_0(\vec{b}; x_i)-\sum_{j=1}^{n} a_j\varphi_j(\vec{b}; x_i)\right]^2 \tag{2}$$

If: $\vec{\Psi}$ = the vector $\in R^m$ with i-component $y_i-\varphi_0(\vec{b}; x_i)$ and Φ = the matrix $\in R^{m \cdot n}$ with $(i-j)$-element $\varphi_j(\vec{b}; x_i)$, the non-linear functional (2) can be written as:

$$r_1(\vec{a},\vec{b})=\|\vec{\Psi}-\Phi\vec{a}\|^2 \tag{3}$$

First, it is proven that it is possible to transform such a separable problem to a minimization problem involving the non-linear parameters only.

THEOREM

Suppose $r_1(\vec{a},\vec{b})$ has a simple isolated minimum for $\vec{b}\in S \subset R^k$ and that the matrix $\Phi(\vec{b})$ is of rank n with continue derivatives in this region for $\vec{b}$. If $\vec{b}$ is constant, the minimum of $r_1(\vec{a},\vec{b})$ is attained for $\vec{a}$ being the solutions of the set of normal equations:

$$(\Phi^T\Phi)\vec{a}=\Phi^T\vec{\Psi} \tag{4}$$

for the corresponding linear regression. This equation can be solved for $\vec{a}$ as:

$$\vec{a}(\vec{b})=(\Phi^T\Phi)^{-1}\Phi^T\vec{\Psi} \tag{5}$$

because of the rank of $(\Phi^T\Phi)$ is the same as the rank of Φ and thus equal n. After putting this result in equation (3) we get the non-linear functional:

$$r_2(\vec{b})=\|\vec{\Psi}-\Phi(\Phi^T\Phi)^{-1}\Phi^T\vec{\Psi}\|^2 \tag{6}$$

which is only function of the non-linear parameters $\vec{b}$. The following theorem is now proven:

If $\hat{\vec{b}}\in S$ is the minimum of $r_2(\vec{b})$ and if is given by equation (5) in which $\Phi=\Phi(\hat{\vec{b}})$ is substituted, then $(\hat{\vec{a}},\hat{\vec{b}})$ is the minimum of $r_1(\vec{a},\vec{b})$.

Proof

One can always find an orthogonal m by m matrix Q, which reduce Φ to his 'trapezoidal' form:

$$Q\Phi=\begin{bmatrix}Q_1\\Q_2\end{bmatrix}\Phi=\begin{bmatrix}U\\0\end{bmatrix} \tag{7}$$

with U a triangular n by n matrix of rank n, and $Q_1 \in R^{n,m}$ and $Q_2 \in R^{m-n,m}$ (see Acton[1]). As a result of the orthogonality of Q, the following relation between Q_1 and Q_2 is obtained:

$$Q^TQ=Q_1^TQ_1+Q_2^TQ_2=I \tag{8}$$

and from equation (7) is found:

$$\Phi=Q^T\begin{bmatrix}U\\0\end{bmatrix} \text{ and } \Phi^T=[U^T0]Q \tag{9}$$

Using these relations one proves easily after some calculations that:

$$\Phi(\Phi^T\Phi)^{-1}\Phi^T=Q^T\begin{bmatrix}I_n & 0\\0 & 0\end{bmatrix}Q=Q_1^TQ_1 \tag{10}$$

and

$$I-\Phi(\Phi^T\Phi)^{-1}\Phi^T=Q_2^TQ_2 \tag{11}$$

For the identity matrices I, we have denoted the rank n as I_n, only where it was necessary.

Out of the last equations it can even be proven that the matrices $Q_1^TQ_1$ and $Q_2^TQ_2$ are idempotent with power 2:

$$\begin{aligned}(Q_1^TQ_1)^2&=Q_1^TQ_1\\(Q_2^TQ_2)^2&=Q_2^TQ_2\end{aligned} \tag{12}$$

Let us now put:

$$\vec{\varepsilon}=\vec{\Psi}-\Phi\vec{a} \tag{13}$$

then the modified functional (6) is given by:

$$r_2(\vec{b})=\vec{\Psi}^TQ_2^TQ_2\vec{\Psi}=\vec{\varepsilon}^TQ_2^TQ_2\vec{\varepsilon} \tag{14}$$

and the primary functional (3) is transformed as:

$$r_1(\vec{a},\vec{b})=\vec{\varepsilon}^T\vec{\varepsilon}=\vec{\varepsilon}^TQ^TQ\vec{\varepsilon}=\vec{\varepsilon}^TQ_1^TQ_1\vec{\varepsilon}+\vec{\varepsilon}^TQ_2^TQ_2\vec{\varepsilon} \tag{15}$$

A combination of equations (14) and (15) results in the following relation between these two functionals:

$$r_1(\vec{a},\vec{b})=r_2(\vec{b})+\vec{\varepsilon}^TQ_1^TQ_1\vec{\varepsilon} \tag{16}$$

The three terms in the above equation are certainly positive, so that:

$$\min_{\vec{a},\vec{b}\in S} r_1(\vec{a},\vec{b})\geqslant \min_{\vec{b}\in S} r_2(\vec{b})+\min_{\vec{a},\vec{b}\in S}\vec{\varepsilon}^TQ_1^TQ_1\vec{\varepsilon} \tag{17}$$

Choosing for $\vec{a}=\vec{a}(\vec{b})=(\Phi^T\Phi)^{-1}\Phi^T\vec{\Psi}$, the second term in the second member of equation (17) is zero, which results in:

$$\min_{\vec{a},\vec{b}\in S} r_1(\vec{a},\vec{b})\geqslant \min_{\vec{b}\in S} r_2(\vec{b}) \tag{18}$$

Otherwise one has always:

$$\min_{\vec{a},\vec{b}\in S} r_1(\vec{a},\vec{b})\leqslant \min_{\substack{\vec{b}\in S\\ \vec{a}=\vec{a}(\vec{b})}} r_1(\vec{a},\vec{b})$$

or with equation (16):

$$\min_{\vec{a},\vec{b}\in S} r_1(\vec{a},\vec{b})\leqslant \min_{\vec{b}\in S} r_2(\vec{b}) \tag{19}$$

The inequalities (18) and (19) prove the theorem.

The minimization problem of the non-linear sum of squares in the $n+k$ parameters of the model (1) is thus reduced to a minimization problem in the k purely non-linear parameters only. Models of the form (1) are used frequently and this reduction of the number of iteration parameters can sometimes improve enormously in computer-time and numerical convergence. Consider now the minimization algorithm for the remaining non-linear parameters.

MINIMIZATION ALGORITHM

To find iteratively the minimum of $r_2(\vec{b})$ a so-called second order method is used. The non-linear functional $r_2(\vec{b})$ in equation (14) is written as:

$$r_2(\vec{b})=\vec{\chi}^T\vec{\chi} \text{ with } \vec{\chi}=Q_2\vec{\Psi}\in R^{m-n} \tag{20}$$

To approximate the minimum value of the objective function $r_2(\vec{b})$ from points $\vec{b}$ near to the minimum $\vec{b}+\overrightarrow{\Delta b}$, the Taylor expansion series with second order terms is used:

$$r_2(\vec{b}+\overrightarrow{\Delta b})=r_2(\vec{b})+\vec{g}\cdot\overrightarrow{\Delta b}+\frac{1}{2}\overrightarrow{\Delta b}^TH\overrightarrow{\Delta b} \tag{21}$$

In this expansion $\vec{g}$ and H are respectively the Jacobian gradient vector and the Hessian matrix. They are defined by:

$$\vec{g}=\left(\frac{\partial r_2}{\partial b}\right)\in R^{1,k} \tag{22}$$

and

$$H=\left(\frac{\partial^2 r_2}{\partial b_i\partial b_j}\quad(i,j=1,k)\right)\in R^{k,k} \tag{23}$$

Our objective is to determine the vector $\overrightarrow{\Delta b}$ of the movement, required to approximate the minimum from $\vec{b}$. To determine $\overrightarrow{\Delta b}$ approximately, consider $\vec{g}$ and H as fixed and differentiate partially the increment:

$$\vec{g}\cdot\overrightarrow{\Delta b}+\frac{1}{2}\overrightarrow{\Delta b}^T\cdot H\cdot\overrightarrow{\Delta b} \tag{24}$$

with respect to $\overrightarrow{\Delta b}$. Setting this result to zero gives:

$$\vec{g}(\vec{b})+H(\vec{b})\cdot\overrightarrow{\Delta b}=0 \tag{25}$$

and after solving for $\overrightarrow{\Delta b}$ yields:

$$\overrightarrow{\Delta b}=-(H(\vec{b}))^{-1}\vec{g}(\vec{b}) \tag{26}$$

as the approximation for the required movement to the minimum $\vec{b}_{min}$ from a point $\vec{b}$ near to the minimum (the current point). Equation (26) is fundamental to all second order solutions for a minimization problem. When it is used directly to generate successive movements toward a minimum from a given initial value b_0, the method is known as the Gauss–Newton algorithm. Direct use of equation (26) is limited, however, because the Hessian matrix H must be computed and inverted at each step of any iterative procedure. If the partial derivation of $r_2(\vec{b})$ is analytically too difficult to perform one can have recourse to numerical derivations, and then several methods to approximate H^{-1} are available. Only one is mentioned.

A first partial differentiation equation (20) gives:

22

$$g_i = \frac{\partial r_2}{\partial b_i} = 2\vec{\chi}^T \frac{\partial \vec{\chi}}{\partial b_i} (i = 1,k) \qquad (27)$$

and a second partial differentiation yields:

$$H_{i,j} = \frac{\partial^2 r_2}{\partial b_i \partial b_j} = 2\frac{\partial \vec{\chi}^T}{\partial b_i}\frac{\partial \vec{\chi}}{\partial b_j} + 2\vec{\chi}^T \frac{\partial^2 \vec{\chi}}{\partial b_i \partial b_j} (i,j = 1,k) \qquad (28)$$

The Newton–Raphson least squares procedure assumes that the second term in equation (28) can be neglected. Therefore we take:

$$\overrightarrow{\Delta b} = -\frac{1}{2} A^{-1} \vec{g} \qquad (29)$$

where A is a symmetric matrix with i-j-element:

$$A_{i,j} = \frac{\partial \vec{\chi}^T}{\partial b_i}\frac{\partial \vec{\chi}}{\partial b_j} (i,j = 1,k) \qquad (30)$$

Finally, we observe the numerical convergence of the method. It can be proven that the matrix H, evaluated at the minimum is positive definite. However, H in equation (26) is not necessarily positive definite, since it is evaluated at a point other than the minimum, so that the process may not converge. This situation is most likely to occur at some distance from the minimum. Moreover, the Hessian H is approximated by the matrix A in equation (30). This is the reason why in some situations it is important firstly to limit the step size (taken as a fraction $\rho_k < 1$) so that a solution is not predicted outside the range of a valid first order approximation to H and secondly to add a positive scalar λ_k to the diagonal elements of A so that $A + \lambda_k I$ is certainly positive definite. Taking this into account, the iteration scheme becomes finally:

$$\vec{b}_{k+1} = \vec{b}_k - \rho_k (A + \lambda_k I_k)^{-1} \vec{g} \qquad (31)$$

The practical determination of the scalars ρ_k and λ_k will be treated in the next paragraph. (We use the index k to mean the kth iteration step. There will be no confusion with the number of non-linear parameters also denoted as k.)

COMPUTATIONAL PROCEDURE

Calculation of $\vec{\chi} = Q_2 \vec{\Psi}$

The determination[1] of the orthogonal matrix Q, which reduces Φ to its trapezoidal form, can best be done using a sequence of Householder transformations. A first transformation $Q^{(1)}$ transforms Φ to a matrix with on the first column all zeros except the first element, a second transformation reduces the second column to all zeros, except the two first numbers etc. This can be visualized as:

$$Q\Phi = \begin{bmatrix} I_{n-1} & 0 \\ 0 & Q^{(n)} \end{bmatrix} \begin{bmatrix} I_{n-2} & 0 \\ 0 & Q^{(n-1)} \end{bmatrix} \cdots \begin{bmatrix} 1 & 0 \\ 0 & Q^{(2)} \end{bmatrix} Q^{(1)}\Phi$$

$$= \begin{bmatrix} x & x & \dots & x \\ 0 & x & & . \\ 0 & 0 & & . \\ \vdots & \vdots & & \vdots \\ 0 & 0 & & 0 \end{bmatrix} \qquad (32)$$

(The zeros in the second member mean zero-matrices of different kind.) Applying the same sequence of transformations on the vector $\vec{\Psi}$, we get the vector $\vec{\chi}$ as the last m–n elements of this result.

Calculation of $\partial\vec{\chi}/\partial b_i$

For the purpose of calculating g_i and $A_{i,j}$ following equations (27) and (30) are needed the derivatives $\partial\vec{\chi}/\partial b_i$. They can be calculated analytically if the derivatives $\partial\varphi_j/\partial b_i$ are determined. It is of course also possible to determine them numerically. The last procedure is less laborious for the user of the program, because no supplementary program is needed to calculate $\partial\varphi_j/\partial b_i$. Yet, it introduces a supplementary inaccuracy in the calculations. If the functions φ_j are sufficiently smooth, it appears that numerical derivation yields no serious risk to lose convergency, but one has to be careful if the functions φ_j are liable to error noise (e.g. results of numerical integrations) .

Scaling of the matrix A in equation (31)

In minimization problems of the sum of squares of deviations the covariance matrix A in the normal equations is usually scaled to obtain a correlation matrix. In this way the normal equations are better conditioned. If

$$A^* = T A T \qquad (33)$$

with T a k by k diagonal matrix with diagonal elements $A_{i,i}^{-1/2}$, then A^* is the scaled correlation matrix. Using equation (33) the increments $\overrightarrow{\Delta b}$ from equation (29) are obtained:

$$\overrightarrow{\Delta b} = -\frac{1}{2} T (A^*)^{-1} T \vec{g} \qquad (34)$$

In order to obtain also for A^* a positive definite matrix, we add to A^* the diagonal matrix $\lambda_k I$, and finally equation (31) is reduced to:

$$\vec{b}_{k+1} = \vec{b}_k - \rho_k T (A^* + \lambda_k I)^{-1} T \vec{g} \qquad (35)$$

Determination of ρ_k and λ_k

Following equation (29) ~~once~~ one can choose $\rho_k = 1/2$ and if necessary a more appropriate ρ_k can be determined with the method of successive division by two, or another line search method. Some authors[2,7] have treated this problem in detail. Here we will try to reduce the number of evaluations of $r_2(\vec{b})$ rather than the number of iteration steps. In order that $A^* + \lambda_k I$ should be positive definite, it is necessary and sufficient to choose $\lambda_k >$ maximum $(0, -e)$, with e the smallest eigenvalue of A^*. It is, however, not necessary to take λ_k too great, because if $\lambda_k \to \infty$ then $\|\overline{\Delta b}\| \to 0$ and the convergence can be slowed down.

In his algorithm, Marquardt[3] has not used an eigenvalue analysis. He starts with a small value for λ_k and takes $\rho_k = 0.5$. Is the kth iteration step successful then λ_{k+1} is set equal λ_k/v $(v > 1)$, if not, the angle between $\overline{\Delta b}$ and $\vec{g}$ is calculated. If this angle is lower than $\pi/4$, then

IF

$$\begin{cases} \rho_{k+1} = \rho_k/2 \\ \lambda_{k+1} = \lambda_k \end{cases} \tag{36}$$

is taken. In the other case:

$$\begin{cases} \rho_{k+1} = \rho_k \\ \lambda_{k+1} = \lambda_k v \end{cases} \tag{37}$$

In our program the eigenvalues are determined with $\rho_k = 1$ and $\lambda_k =$ maximum $(0, -e)$ with e the smallest eigenvalue. If one iteration step is not successful, e.g. the kth step, ρ_k and λ_k are transformed following equation (36). But if ρ_k becomes smaller than 0.03, the direction is changed, with $\rho_{k+1} = 1$ and λ is transformed as follows:

$$\begin{cases} \lambda_{k+1} = 2\lambda_k (\text{if } \lambda_k \neq 0) \\ \lambda_{k+1} = e \ (\text{if } \lambda_k = 0) \end{cases} \tag{38}$$

The inverse of $(A^* + \lambda_k I)$

Let the eigenvalues and the eigenvectors of A^* be denoted by e_j and v_j $(j = 1, \ldots k)$ respectively, then we have:

$$(A^*)^{-1} = \sum_{j=1}^{k} e_j^{-1} v_j v_j^{\mathrm{T}} \tag{39}$$

The eigenvectors of $A^* + \lambda_k I$ are the same as those of A^*, but the eigenvalues of this matrix are given by $e_j + \lambda_k$, so that:

$$(A^* + \lambda_k I)^{-1} = \sum_{j=1}^{k} (e_j + \lambda_k)^{-1} v_j v_j^{\mathrm{T}} \tag{40}$$

If it is necessary to test several values for the parameter λ_k (see above), this procedure seems to be very interesting, because we don't need any matrix inversion.

Calculation of the linear parameters

After the minimization of $r_2(\vec{b})$ the linear parameters $\vec{a}(\vec{b})$ given by equation (4) can be calculated in an easy way[7]. Using equation (9), equation (4) is transformed in:

$$[U^{\mathrm{T}} 0] Q Q^{\mathrm{T}} \begin{bmatrix} U \\ 0 \end{bmatrix} \vec{a} = [U^{\mathrm{T}} 0] Q \vec{\Psi}$$

or

$$U \vec{a} = Q_1 \vec{\Psi} \tag{41}$$

Because U is a triangular matrix, this set of equations is easily solved for $\vec{a}$.

Stopcriterium

If $r_2(\vec{b}_k)$ is the value of r_2 after k iterations, and if $k+1$ is a successful iteration than $\vec{b}_{k+1}$ is taken as a local minimum if:

$$\frac{r_2(\vec{b}_k) - r_2(\vec{b}_{k+1})}{r_2(\vec{b}_k)} < \varepsilon \tag{42}$$

with ε a predefined small number, given by the user of the program. In order to take action in a case of non-convergence, the user of the program must also give a value for the maximum number of iterations.

LISTING OF THE COMPUTER PROGRAMS

The above algorithm can be implemented in a computer program as follows. First, a main subroutine is needed which determines the minimum of $r_2(\vec{b})$ and the corresponding parameters $\vec{a}$ and $\vec{b}$ of the regression model. For this subroutine which is named 'BBO3M2' a flowchart can be drawn as shown in Fig. 1. The variables have been labeled as in the text as much as possible. This main subroutine requires two other subroutines. A first one which is named 'BBO3EI' determines the eigenvalues and the eigenvectors of a real symmetric matrix, and a second one which is named 'BBO3TH' reduces a general m by n matrix to his trapezoidal form using a series of orthogonal transformations. In the flowchart the subroutine 'BBO3TH' is needed in the boxes denoted by '*'. This subroutine 'BBO3TH' as well as the subroutine 'BBO3EI' are, of course, standard routines; they have been copied

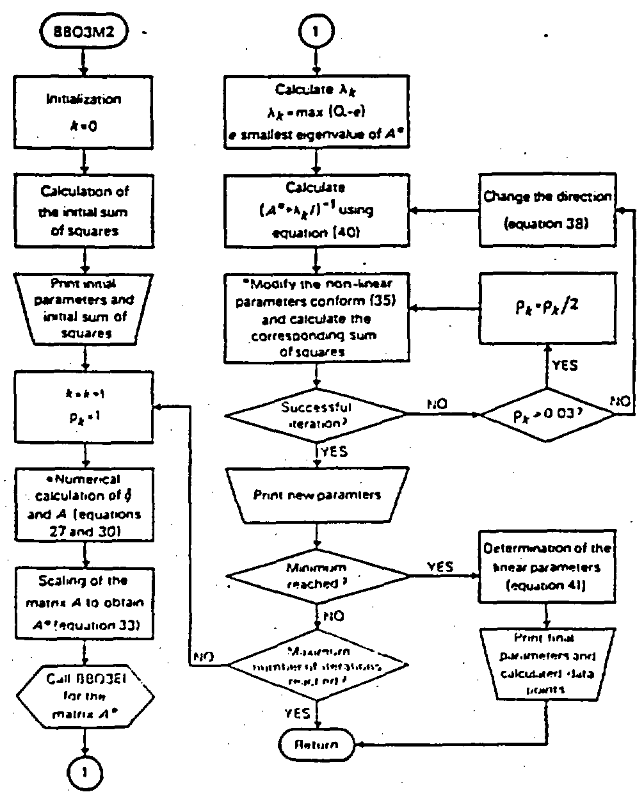

Figure 1

from the Scientific Subroutine Package (SSP-library) of IBM. All programs are written in Fortran IV.

```
      SUBROUTINE BB03N2(A,ALIN,X,Y,M,N,K,MIT,EPS)
C
C     ..................................................................
C
C     SUBROUTINE BB03N2
C
C     PURPOSE
C        TO PERFORM A GENERAL LEAST SQUARES ESTIMATION OF NON-LINEAR
C        PARAMETERS
C
C     USAGE
C        CALL BB03N2(A,ALIN,X,Y,M,N,K,MIT,EPS)
C
C     DESCRIPTION OF THE PARAMETERS
C        A : DOUBLE PRECISION  VECTOR OF DIMENSION K, WHICH CONTAINS
C        THE INITIAL NONLINEAR PARAMETER  ESTIMATIONS. ON RETURN THIS
C        VECTOR CONTAINS THE FINAL NONLINEAR PARAMETER ESTIMATIONS.
C        ALIN : DOUBLE PRECISION OUTPUT VECTOR OF DIMENSION N,CONTAINING
C        THE LINEAR PARAMETERS
C        X: DOUBLE PRECISION VECTOR OF DIMENSION M, WHICH CONTAINS
C        THE DATA OF THE INDEPENDENT VARIABLE
C        Y : DOUBLE PRECISION VECTOR OF DIMENSION M,WHICH CONTAINS
C        THE DATA OF THE DEPENDENT VARIABLE
C        M: NUMBER OF DATA POINTS(MAXIMUM 50)
C        N : NUMBER OF LINEAR PARAMETERS(MAXIMUM 10)
C        K : NUMBER OF NON-LINEAR PARAMETERS
C        MIT : MAXIMUM NUMBER OF ITERATIONS ALLOWED
C        EPS : DOUBLE PRECISION INPUT PARAMETER. THE ITERATION STOPS
C        IF THE RELATIVE CHANGEMENT OF THE SUM OF SQUARES IS
C        LOWER THAN EPS.
C
C     SUBROUTINES REQUIRED
C        BB03UF : MUST BE FURNISHED BY THE USER
C        NO3EI : CALCULATES THE EIGENVALUES OF A REAL SYMMETRIC MATRIX
C        BB03TH : TRANSFORMS A MATRIX TO HIS TRAPEZIDAL FORM,USING
C        HOUSEHOLDER TRANSFORMATIONS
C
C     REMARKS
C        1) FOR PROBLEMS WHERE M IS GREATER THAN 50 OR N IS GREATER
C        THAN 10,ONLY THE DIMENSION STATEMENTS HAVE TO BE ADAPTED
C        2) THE PROGRAM IS WRITTEN IN DOUBLE PRECISION
C
C     ..................................................................
C
C
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION A(1),ALIN(1),X(1),Y(1)
      DIMENSION PSI(50),PSIA(50),AJ(50,10)
      DIMENSION FI(50,11),FINUL(50),AN(60)
     *,G(10),E(10),AK(10),H(100),DA(10)
      EQUIVALENCE(FI(1,11),FINUL(1)),(H(1),AJ(1,1))
C
C     NIT : NUMBER OF ITERATIONS
C
      NIT=0
C
C     CALCULATION OF THE INITIAL SUM OF SQUARES
      CALL BB03UF(A,X,FI,M,N)
      DO 1 I=1,M
    1 PSI(I)=Y(I)-FINUL(I)
      CALL BB03TH(M,N,FI,PSI)
      SSN=0.
      MT=N+1
      STEP=1.
      DO 2 I=MT,M
    2 SSN=SSN+PSI(I)**2
      WRITE(3,3) SSN,(A(I),I=1,K)
    3 FORMAT(//,' INITIAL SUM OF SQUARES=',E15.5,
     */,10X,'NON-LINEAR PARAMETERS=',5E15.5,/,32X,5E15.5)
C
C     NUMERICAL CALCULATION OF THE DERIVATIVES(EQUATIONS (3.8) AND (3.11)
C
   24 DO 4 J=1,K
      B=A(J)
      G(J)=0.
      DEL=B*0.005
      IF(DEL.EQ.0.D0) DEL=0.005
      A(J)=B+DEL
      CALL BB03UF(A,X,FI,M,N)
      A(J)=B
      DO 5 I=1,M
    5 PSIA(I)=Y(I)-FINUL(I)
      CALL BB03TH(M,N,FI,PSIA)
      DO 6 I=MT,M
      IT=I-N
      AJ(IT,J)=(PSIA(I)-PSI(I))/DEL
    6 G(J)=G(J)+AJ(IT,J)*PSI(I)
    4 CONTINUE
C
C     SCALING OF THE MATRIX A(SEE EQUATION (4.2))
C
      MN=M-N
      IS=0
      DO 7 I=1,K
      DO 8 J=1,I
      IS=IS+1
      SUM=0.
      DO 9 IN=1,MN
    9 SUM=SUM+AJ(IN,I)*AJ(IN,J)
    8 AN(IS)=SUM
    7 E(I)=DSQRT(SUM)
      IS=0
      DO 11 I=1,K
      DO 10 J=1,I
      IS=IS+1
      IF(E(I)*E(J).EQ.0.) GO TO 10
      AN(IS)=AN(IS)/(E(I)*E(J))
   10 CONTINUE
      IF(E(I).EQ.0.) GO TO 11
      G(I)=G(I)/E(I)
   11 CONTINUE
C
C     CALCULATION OF THE EIGENVALUES AND EIGENVECTORS OF THE
C     SCALED MATRIX AN
C
      CALL NO3EI(AN,H,K,0)
C
C     TEST IF THE DETERMINANT OF THE MATRIX AN IS NOT ZERO
C
      LI=0
      DO 106 I=1,K
      LI=LI+I
      IF(AN(LI).NE.0.) GO TO 106
      WRITE(3,100)
  100 FORMAT('  THE ITERATION PROCESS HAS STOPPED',/,
     1        '  THE DETERMINANT OF AN INVERTING MATRIX IS ZERO',/,
     2    '  TRY OTHER STARTING VALUES')
      GO TO 107
  106 CONTINUE
C
C     INITIAL VALUE OF LAMBDA(VARIABLE DL)
C
      EMIN=AN(IS)
      DL=0.
      IF(EMIN.LE.0.D0) DL=-EMIN
C
C     CALCULATION OF THE INVERSE OF THE SCALED MATRIX A* USING THE
C     EIGENVALUES AND THE EIGENVECTORS(SEE EQUATION (4.9))
C
   38 DO 12 I=1,K
      SOM=0.
      DO 13 J=1,K
      SUM=0.
      DO 14 L=1,K
      LI=(L-1)*K+I
      LJ=(L-1)*K+J
      LL=L*(L+1)/2
   14 SUM=SUM+H(LI)*H(LJ)/(AN(LL)+DL)
      SUM=SUM*G(J)
   13 SOM=SOM+SUM
      DA(I)=-SOM
      IF(E(I).EQ.0.) GO TO 12
      DA(I)=-SOM/E(I)
   12 CONTINUE
C
C     MODIFICATION OF THE NONLINEAR PARAMETERS AND CALCULATION OF THE
C     CORRESPONDING SUM OF SQUARES(SEE EQUATION (4.4))
C
   19 DO 18 I=1,K
   18 AN(I)=A(I)+DA(I)*STEP
      CALL BB03UF(AN,X,FI,M,N)
      DO 15 I=1,M
   15 PSI(I)=Y(I)-FINUL(I)
      CALL BB03TH(M,N,FI,PSI)
      SSNN=0.
      DO 16 I=MT,M
   16 SSNN=SSNN+PSI(I)*PSI(I)
C
C     TESTING IF THE ITERATION IS SUCCESSFUL OR NOT AND IF THE MAXIMUM
C     NUMBER OF ITERATIONS OR THE MINIMUM IS NOT YET REACHED.
C     IF NECESSARY AND(VARIABLE STEP) AND LAMBDA(VARIABLE DL)
C     ARE CHANGED
C
      IF(SSNN.LT.SSN) GOTO 17
      IF(STEP.GT.0.03) GOTO 36
      STEP=1.
      DL=DL*DL
      IF(DL.EQ.0.) DL=EMIN
      GOTO 38
   36 STEP=STEP*0.5
      GOTO 19
   17 WRITE(3,26)SSNN,(AN(I),I=1,K)
   26 FORMAT(/,' SUCCESSFUL ITERATION ',
     1/,10X,' SUM OF SQUARES=',E15.5,10X,
     */,10X,'NON-LINEAR PARAMETERS=',5E15.5,/,32X,5E15.5)
   32 DO 22 I=1,K
   22 A(I)=AN(I)
      IF(SSNN.LT.1.D-7) GO TO 40
      IF(DABS(SSN-SSNN)/SSN.GT.EPS) GO TO 20
   40 WRITE(3,27)
   27 FORMAT(' ITERATION NORMALLY ENDED   ')
      GOTO 23
   20 NIT=NIT+1
      IF(NIT.GE.MIT) GOTO 21
      SSN=SSNN
      STEP=1.
      GOTO 24
   21 WRITE(3,28)
   28 FORMAT(' THE MAXIMUM NUMBER OF ITERATIONS IS REACHED ')
C
C     DETERMINATION OF THE FINAL LINEAR PARAMETERS(SEE EQUATION (4.10))
C
   23 IF(N.EQ.0) GOTO 39
      DO 31 I=1,N
      DL=FI(I,I)
      PSI(I)=PSI(I)/DL
      DO 31 J=I,N
   31 FI(I,J)=FI(I,J)/DL
      DO 32 II=1,N
      I=N-II+1
      ALIN(I)=PSI(I)
      IF(I.EQ.1) GOTO 33
      IM1=I-1
      DO 32 J=1,IM1
   32 PSI(J)=PSI(J)-ALIN(I)*FI(J,I)
   33 CONTINUE
      WRITE(3,29) (ALIN(I),I=1,N)
   29 FORMAT(' LINEAR PARAMETERS=',6E15.5,/,19X,6E15.4)
C
C     OUTPUT OF THE DATA-POINTS
C
   39 CALL BB03UF(A,X,FI,M,N)
      WRITE(3,99)
   99 FORMAT(///,5X, 'X-VALUES',14X,'Y-VALUES',4X,
     1 'ESTIMATED Y-VALUES',12X,'DEVIATIONS',/)
      DO 95 I=1,M
      SOM=FINUL(I)
      IF(N.EQ.0) GOTO 25
      DO 35 J=1,N
   35 SOM=SOM+ALIN(J)*FI(I,J)
   25 DEV=Y(I)-SOM
   95 WRITE(3,30) X(I),Y(I),SOM,DEV
   30 FORMAT(F13.3,3F24.3)
  107 RETURN
      END
```

```
      SUBROUTINE NO3EI(A,R,N,MV)
C
C     ..................................................................
C
C        SUBROUTINE NO3EI
C
C        PURPOSE
C           COMPUTE EIGENVALUES AND EIGENVECTORS OF A REAL SYMMETRIC
C           MATRIX
C
C        USAGE
C        CALL NO3EI(A,R,N,MV)
C
C        DESCRIPTION OF PARAMETERS
C
C           A - ORIGINAL MATRIX (SYMMETRIC), DESTROYED IN COMPUTATION.
C               RESULTANT EIGENVALUES ARE DEVELOPED IN DIAGONAL OF
```

```fortran
C              MATRIX A IN DESCENDING ORDER.
C           R - RESULTANT MATRIX OF EIGENVECTORS (STORED COLUMNWISE,
C              IN SAME SEQUENCE AS EIGENVALUES)
C           N - ORDER OF MATRICES A AND R
C           MV- INPUT CODE
C                   0   COMPUTE EIGENVALUES AND EIGENVECTORS
C                   1   COMPUTE EIGENVALUES ONLY (R NEED NOT BE
C                       DIMENSIONED BUT MUST STILL APPEAR IN CALLING
C                       SEQUENCE)
C
C        REMARKS
C           ORIGINAL MATRIX A MUST BE REAL SYMMETRIC (STORAGE MODE=1)
C           MATRIX A CANNOT BE IN THE SAME LOCATION AS MATRIX R
C
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED
C           NONE
C
C        METHOD
C           DIAGONALIZATION METHOD ORIGINATED BY JACOBI AND ADAPTED
C           BY VON NEUMANN FOR LARGE COMPUTERS AS FOUND IN 'MATHEMATICAL
C           METHODS FOR DIGITAL COMPUTERS', EDITED BY A. RALSTON AND
C           H.S. WILF, JOHN WILEY AND SONS, NEW YORK, 1962, CHAPTER 7
C
C     ..................................................................
C
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION A(1),R(1)
C
C        ...............................................................
C
C        GENERATE IDENTITY MATRIX
C
    5 RANGE=1.0D-10
      IF(MV-1) 10,25,10
   10 IQ=-N
      DO 20 J=1,N
      IQ=IQ+N
      DO 20 I=1,N
      IJ=IQ+I
      R(IJ)=0.0
      IF(I-J) 20,15,20
   15 R(IJ)=1.0
   20 CONTINUE
C
C        COMPUTE INITIAL AND FINAL NORMS (ANORM AND ANORMX)
C
   25 ANORM=0.0
      DO 35 I=1,N
      DO 35 J=I,N
      IF(I-J) 30,35,30
   30 IA=I+(J*J-J)/2
      ANORM=ANORM+A(IA)*A(IA)
   35 CONTINUE
      IF(ANORM) 165,165,40
   40 ANORM=1.414*DSQRT(ANORM)
      ANRMX=ANORM*RANGE/FLOAT(N)
C
C        INITIALIZE INDICATORS AND COMPUTE THRESHOLD, THR
C
      IND=0
      THR=ANORM
   45 THR=THR/FLOAT(N)
   50 L=1
   55 M=L+1
C
C        COMPUTE SIN AND COS
C
   60 MQ=(M*M-M)/2
      LQ=(L*L-L)/2
      LM=L+MQ
   62 IF(DABS(A(LM))-THR) 130,65,65
   65 IND=1
      LL=L+LQ
      MM=M+MQ
      X=0.5*(A(LL)-A(MM))
   68 Y=-A(LM)/DSQRT(A(LM)*A(LM)+X*X)
      IF(X) 70,75,75
   70 Y=-Y
   75 SINX=Y/DSQRT(2.0*(1.0+(DSQRT(1.0-Y*Y))))
      SINX2=SINX*SINX
   78 COSX=DSQRT(1.0-SINX2)
      COSX2=COSX*COSX
      SINCS =SINX*COSX
C
C        ROTATE L AND M COLUMNS
C
      ILQ=N*(L-1)
      IMQ=N*(M-1)
      DO 125 I=1,N
      IQ=(I*I-I)/2
      IF(I-L) 80,115,80
   80 IF(I-M) 85,115,90
   85 IM=I+MQ
      GO TO 95
   90 IM=M+IQ
   95 IF(I-L) 100,105,105
  100 IL=I+LQ
      GO TO 110
  105 IL=L+IQ
  110 X=A(IL)*COSX-A(IM)*SINX
      A(IM)=A(IL)*SINX+A(IM)*COSX
      A(IL)=X
  115 IF(MV-1) 120,125,120
  120 ILR=ILQ+I
      IMR=IMQ+I
      X=R(ILR)*COSX-R(IMR)*SINX
      R(IMR)=R(ILR)*SINX+R(IMR)*COSX
      R(ILR)=X
  125 CONTINUE
      X=2.0*A(LM)*SINCS
      Y=A(LL)*COSX2+A(MM)*SINX2-X
      X=A(LL)*SINX2+A(MM)*COSX2+X
      A(LM)=(A(LL)-A(MM))*SINCS+A(LM)*(COSX2-SINX2)
      A(LL)=Y
      A(MM)=X
C
C        TESTS FOR COMPLETION
C
C        TEST FOR M = LAST COLUMN
C
  130 IF(M-N) 135,140,135
  135 M=M+1
      GO TO 60
C
C        TEST FOR L = SECOND FROM LAST COLUMN
C
  140 IF(L-(N-1)) 145,150,145
  145 L=L+1
      GO TO 55
  150 IF(IND-1) 160,155,160
  155 IND=0
      GO TO 50
C
C        COMPARE THRESHOLD WITH FINAL NORM
C
  160 IF(THR-ANRMX) 165,165,45
C
C        SORT EIGENVALUES AND EIGENVECTORS
C
  165 IQ=-N
      DO 185 I=1,N
      IQ=IQ+N
      LL=I+(I*I-I)/2
      JQ=N*(I-2)
      DO 185 J=I,N
      JQ=JQ+N
      MM=J+(J*J-J)/2
      IF(A(LL)-A(MM)) 170,185,185
  170 X=A(LL)
      A(LL)=A(MM)
      A(MM)=X
      IF(MV-1) 175,185,175
  175 DO 180 K=1,N
      ILR=IQ+K
      IMR=JQ+K
      X=R(ILR)
      R(ILR)=R(IMR)
  180 R(IMR)=X
  185 CONTINUE
      RETURN
      END
```

```fortran
      SUBROUTINE BBO3TH(M,N,FI,PSI)
C
C     ..................................................................
C
C     SUBROUTINE BBO3TH
C
C     PURPOSE
C        TO PERFORM A GENERAL M BY N MATRIX FI TO HIS TRAPEZOIDAL FORM,
C        USING HOUSEHOLDER ORTHOGONAL TRANSFORMATIONS. THE SAME
C        TRANSFORMATIONS ARE PERFORMED ON THE VECTOR PSI.
C
C     USAGE
C     CALL BBO3TH(M,N,FI,PSI)
C
C     DESCRIPTION OF THE PARAMETERS
C        M : NUMBER OF ROWS OF MATRIX FI
C        N : NUMBER OF COLUMNS OF MATRIX FI
C        FI : DOUBLE PRECISION 50 BY 11 INPUT MATRIX. ON RETURN FI
C        CONTAINS THE TRAPEZOIDAL FORM
C        PSI : DOUBLE PRECISION VECTOR OF DIMENSION 50,ON WHICH THE
C        SAME TRANSFORMATIONS ARE PERFORMED
C
C     SUBROUTINES REQUIRED
C        NONE
C
C     METHOD
C        HOUSEHOLDER ORTHOGONAL TRANSFORMATIONS
C
C     REMARKS
C        1) FOR PROBLEMS WHERE M IS GREATER THAN 50 OR N IS GREATER
C        THAN 11, ONLY THE DIMENSION STATEMENTS HAVE TO BE ADAPTED
C        2) THE PROGRAM IS WRITTEN IN DOUBLE PRECISION
C
C
C     ..................................................................
C
C
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION FI(50,11),W(50),PSI(50)
      IF(N.EQ.0) RETURN
      DO 1 I=1,N
      SUM=0.
      DO 2 J=I,M
    2 SUM=SUM+FI(J,I)*FI(J,I)
      S=DSQRT(SUM)
      IF(FI(I,I).LT.0.) S=-S
      TK2=S*(S+FI(I,I))
      IF(TK2.EQ.0.) GO TO 1
      DO 10 J=I,M
   10 W(J)=FI(J,I)
      W(I)=W(I)+S
      T=0.
      DO 3 J=I,M
    3 T=T+W(J)*PSI(J)
      T=T/TK2
      DO 4 J=I,M
    4 PSI(J)=PSI(J)-W(J)*T
      DO 5 J=I,N
      T=0.
      DO 6 K=I,M
    6 T=T+W(K)*FI(K,J)
      T=T/TK2
      DO 7 K=I,M
    7 FI(K,J)=FI(K,J)-W(K)*T
    5 CONTINUE
    1 CONTINUE
    8 RETURN
      END
```

AN EXAMPLE

For each problem the user of the above subroutines has to furnish himself two Fortran programs. The first one is the main program, in which the subroutine 'BBO3M2' is called after that the data-points (x_i, y_i) are read in or generated. The second one is a subroutine BBO3UF (A,X,FI,M,N), in which the terms $\varphi_j(\vec{b}; x)$ of the fitting function φ are generated for given non-linear parameter-values $\vec{b}$. In this subroutine the first argument A contains these non-linear parameters, the second argument X contains the x-values of the data-points, while the last two ones M and N respectively denote the number of data-points and the number of non-linear parameters. In the elements $FI(I,J)$ of the matrix FI (50,11) the terms $\varphi_j(\vec{b}; x_i)$

with corresponding indices have to be stored. The special values $\varphi_0(\vec{b}; x_i)$ have always to be programmed in the elements FI (I,11). If there is no function $\varphi_0(\vec{b}; x)$ the elements FI (I,11) must be put zero. The above described program has been tested for several regression models. We mention only one.

As example 50 data-points (x_i, y_i) have been generated from the equation:

$$y = a_1 + a_2 th[b_1(\log x - b_2)] \tag{43}$$

with parameter-values:

$$a_1 = 200, \quad a_2 = 150, \quad b_1 = 3, \quad b_2 = 1$$

and with:

$$x_i = 0.2, 0.4, 0.6, \ldots, 10$$

This regression model contains two non-linear parameters (b_1, b_2) and two linear parameters (a_1, a_2) with corresponding functions:

$$\varphi_1(\vec{b}; x) = 1$$

$$\varphi_2(\vec{b}; x) = th[b_1(\log x - b_2)] \tag{44}$$

There is no function $\varphi_0(\vec{b}; x)$. Starting from the initial estimations (7., 2.) for the non-linear parameters (b_1, b_2) the proposed program has been used to fit the model (43) to the generated data-points. The main program and the subroutine BBO3UF which are needed for this problem are listed below.

```
      PROGRAM BBO3.P
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION X(50),Y(50),ALIN(2),A(2)
      M=50
      K=2
      N=2
      DO 10 I=1,M
      X(I)=I*0.2
   10 Y(I)=200.D0+150.D0*DTANH(3.D0*(DLOG(X(I))-1.D0))
      A(1)=7.
      A(2)=2.
      CALL BBO3M2(A,ALIN,X,Y,M,N,K,30,0.0005)
      STOP
      END
```

```
      SUBROUTINE BBO3UF(A,X,FI,K,M)
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION A(1),X(1),FI(50,11)
      DO 1 I=1,M
      FI(I,11)=0.
      FI(I,1)=1.
    1 FI(I,2)=DTANH(A(1)*(DLOG(X(I))-A(2)))
      RETURN
      END
```

RESULTS OF THE PROGRAM

```
INITIAL SUM OF SQUARES=     0.31716D 06
        NON-LINEAR PARAMETERS=     0.70000D 01     0.20000D 01

SUCCESSFUL ITERATION
        SUM OF SQUARES=     0.35170D 06
        NON-LINEAR PARAMETERS=    -0.21439D 01     0.19449D 01

SUCCESSFUL ITERATION
        SUM OF SQUARES=     0.11515D 06
        NON-LINEAR PARAMETERS=     0.20673D-01     0.20574D 01

SUCCESSFUL ITERATION
        SUM OF SQUARES=     0.97203D 05
        NON-LINEAR PARAMETERS=     0.31019D 00     0.26544D 01

SUCCESSFUL ITERATION
        SUM OF SQUARES=     0.84391D 05
        NON-LINEAR PARAMETERS=     0.42823D 00     0.10628D 01

SUCCESSFUL ITERATION
        SUM OF SQUARES=     0.49558D 05
        NON-LINEAR PARAMETERS=     0.77144D 00     0.43024D 00

SUCCESSFUL ITERATION
        SUM OF SQUARES=     0.31636D 05
        NON-LINEAR PARAMETERS=     0.14030D 01     0.12609D 01

SUCCESSFUL ITERATION
        SUM OF SQUARES=     0.11628D 05
        NON-LINEAR PARAMETERS=     0.19084D 01     0.88434D 00

SUCCESSFUL ITERATION
        SUM OF SQUARES=     0.12741D 04
        NON-LINEAR PARAMETERS=     0.24157D 01     0.13234D 01

SUCCESSFUL ITERATION
        SUM OF SQUARES=     0.12970D 02
        NON-LINEAR PARAMETERS=     0.29461D 01     0.99734D 00

SUCCESSFUL ITERATION
        SUM OF SQUARES=     0.11144D-02
        NON-LINEAR PARAMETERS=     0.29998D 01     0.10030D 01

SUCCESSFUL ITERATION
        SUM OF SQUARES=     0.27261D-07
        NON-LINEAR PARAMETERS=     0.30000D 01     0.10000D 01
ITERATION NORMALLY ENDED
LINEAR PARAMETERS=     0.20000D 03     0.15000D 03
```

X-VALUES	Y-VALUES	ESTIMATED Y-VALUES	DEVIATIONS
0.200	50.000	50.000	0.000
0.400	50.003	50.003	0.000
0.600	50.035	50.035	0.000
0.800	50.195	50.195	0.000
1.000	50.742	50.742	0.000
1.200	52.204	52.204	0.000
1.400	55.497	55.497	0.000
1.600	61.978	61.978	-0.000
1.800	73.326	73.326	-0.000
2.000	91.376	91.376	-0.000
2.200	115.615	115.615	-0.000
2.400	146.413	146.413	-0.000
2.600	180.094	180.094	-0.000
2.800	213.246	213.246	-0.000
3.000	243.125	243.125	0.000
3.200	268.047	268.047	0.000
3.400	287.878	287.878	0.000
3.600	303.093	303.093	0.000
3.800	314.553	314.553	0.000
4.000	323.101	323.101	0.000
4.200	329.460	329.460	0.000
4.400	334.199	334.199	0.000
4.600	337.747	337.747	0.000
4.800	340.423	340.423	0.000
5.000	342.449	342.449	0.000
5.200	344.001	344.001	0.000
5.400	345.197	345.197	0.000
5.600	346.126	346.126	0.000
5.800	346.856	346.856	-0.000
6.000	347.428	347.428	-0.000
6.200	347.886	347.886	-0.000
6.400	348.249	348.249	-0.000
6.600	348.543	348.543	-0.000
6.800	348.781	348.781	-0.000
7.000	348.975	348.975	-0.000
7.200	349.134	349.134	-0.000
7.400	349.265	349.265	-0.000
7.600	349.373	349.373	-0.000
7.800	349.464	349.464	-0.000
8.000	349.539	349.539	-0.000
8.200	349.602	349.602	-0.000
8.400	349.654	349.654	-0.000
8.600	349.701	349.701	-0.000
8.800	349.740	349.740	-0.000
9.000	349.772	349.772	-0.000
9.200	349.801	349.801	-0.000
9.400	349.825	349.825	-0.000
9.600	349.845	349.845	-0.000
9.800	349.863	349.863	-0.000
10.000	349.879	349.879	-0.000

From the computer results one can verify the very rapid convergency from the chosen initial estimates for b_1 and b_2 towards the exactly optimal values. Note also that the linear parameters are updated only at the very last iteration step, so that an initial choice is not needed for the procedure. Of particular interest is the obtained convergency speed and the ease with which the method can be applied. This has certainly two reasons: first the linear and the non-linear parameters have been separated and second the number of computation steps are reduced due to the fact that the inverses of matrices of the form $A + \lambda I$ have been calculated with the eigenvalues and eigenvectors.

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