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USE OF A GENERAL NONLINEAR LEAST-SQUARES
CURVE FITTING PROGRAM WITH NONCLOSED
FORM RELATIONSHIPS

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MASTER

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USE OF A GENERAL NONLINEAR LEAST-SQUARES CURVE FITTING PROGRAM WITH
NONCLOSED FORM RELATIONSHIPS

ABSTRACT

A use for GNLS, a general nonlinear least-squares curve fitting program is presented. In this use GNLS determines a set of best parameters for relationships that cannot be written in closed form. This program can be useful for experimenters who need to determine experimental parameters by fitting non-closed form relationships to experimental data. Two examples are given to indicate how GNLS can be used for this type of problem.

INTRODUCTION

GNLS is a general nonlinear least-squares curve fitting routine. The history of GNLS has been lost in time, and only folklore remains to tell of its origin. F.J.Ackerman published UCID 15636 (Ref.1) in 1970 to make GNLS generally available here at Lawrence Livermore Laboratory (LLL). Along with many others, I have used this program for a number of years to determine the parameters of an arbitrary function (selected by the user) by a least-squares fit of the function to a set of input data.

The usual version of GNLS allows one dependent variable (Y), and up to five independent variables (X), 20 parameters(P) to be fitted, and 20 constants (C). The number of parameters and constants can be increased if necessary. (If you used more than 20 parameters to fit your data, you may need

1. F. J. Ackerman, GNLS: A Computer Program for General Nonlinear Least-Squares Curve Fitting, Lawrence Livermore Laboratory, Livermore, CA, UCID-15636 (1970).

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to look closely at the function you are using.) The functional relationship can be written¹:

$$Y = f(C_1, C_2, \dots C_l, P_1, P_2, \dots P_m, X_1, X_2, \dots X_n). \quad (1)$$

In most uses of GNLS that I know, the function f has been a straightforward mathematical function. For example,

$$Y = \sum_{i=1}^5 C_i \cdot \sin(X_2 \cdot P_1) + (C_{20-i} \cdot X_1) + \sum_{i=4}^{10} C_{i+2} \cdot \sinh(X_3 \cdot P_{i-1}). \quad (2)$$

HOW GNLS WORKS

About five years ago I needed to adjust 12 parameters in a computer model that calculated the pressure-volume relationship for porous rocks. My attempts to do this by trial and error turned out to be mostly error. Because of this I looked into using GNLS to fit the model to the experimental data. I concluded that GNLS compares a set of numbers calculated using several parameters pair-wise with an input set of numbers. GNLS then varies in an orderly manner the parameters used in calculating the numbers so that the sum of the squares of the pair differences is a minimum.* In other words, how the calculated numbers are obtained is of little concern to GNLS.

A function like the one in Eq. (2) can be replaced by any model that generates a set of numbers that depend on a set of parameters. The entity that replaces the function will be termed a model for the remainder of this report.

*GNLS can also use other fitting criteria.

The use of GNLS has an additional bonus for the experimenter: there is no need to understand how the parameters are varied by GNLS; one needs only to understand the model that is used.

The conclusion reached in the first paragraph of this section was very useful, since GNLS would consider my 1500-card computer model in exactly the same manner as a mathematical function. This fact did not, of course, remove the problem of uniqueness of the determined parameters. But this approach did save countless hours at the TTY and gave a better fit than generally possible by the trial and error method.

CONSTRUCTING A MODEL FOR GNLS

I used GNLS with this approach on one other problem and again had excellent results. The nonlinear least-squares curve fitting program does not appear to be in wide use among experimenters. I believe it could be very useful in a number of experiments where the data cannot easily be fitted to a closed form mathematical function. I will illustrate with a couple of examples the steps (in some cases tricks) needed to get a model to a form that GNLS likes.

EXAMPLE 1

The arbitrary function used in GNLS is calculated in a subroutine called CALCY. A typical CALCY is of the form:

```
SUBROUTINE CALCY
USE SKINNEY**
DO 1 I = 1, ND
1  CY(I) = C(1)*EXPF(P(1)*X(I,1))+C(2)*P(2)*SINH(X(I,2))
RETURN
END
```

All input data, constants, and starting parameters are read in main and

**Shorthand way of using common and dimension statements.

passed back and forth with CALCY in a common statement. The use of GNLS therefore reduces to writing CALCY in a form acceptable to GNLS.

My approach in constructing a CALCY has been to write a program to calculate the model with a given set of parameters. When the program is completed, I form subroutine CALCY. This approach makes it easier to debug and to verify the model and the computer code. As most people do, I customarily write my programs using variable names that relate to some meaning; I must set the relationships between my variables and the GNLS parameters. This is the first step in CALCY, and is illustrated in Fig. 1 for the porous rock pressure-volume model.

The numbers calculated in CALCY are passed to main as CY(I). The last step in CALCY is, therefore, to set the CY(I) equal to the numbers calculated by the model, thereby allowing GNLS to compare the CY(I) with the input data.

As GNLS requires a one-to-one relationship between the independent and dependent variables, it is necessary in many cases to rearrange the input data to have this one-to-one relationship. An example of this rearrangement is the data for the pressure-volume model. The volume is a double-valued function of the pressure (i.e., different values for increasing pressure and decreasing pressure). Differing values are unsuitable for GNLS. The fix was easy. Order the input data so that for volumes (V) during increasing pressure (P): $V(P) = f(P)$, and for volumes during decreasing pressure: $V(P) = f(2.0 P_{\max} - P)$. This input setup is shown in Fig. 2. A corresponding reverse relationship must be made in CALCY in order to correlate the numbers, CY(I), passed to main.

EXAMPLE 2

As a second example of an input GNLS problem, consider an experiment in which heat flows radially outward in a cylindrical sample. At several radii, thermocouples measure the temperatures at a set of times. I want to determine the thermal diffusivity from these data.

The partial differential equation is approximated in the usual manner in CALCY with a series of concentric rings and a relatively small time step. Two problems are encountered. First, there are n (the number of thermocouples) dependent variables (the temperatures at the various thermocouple locations) for the independent variable (time). Second, the positions of the thermo-

```

RMINI=ABS(P(1))
RMAXI=ABS(P(2))
RMINN=ABS(P(3))
RMAXN=ABS(P(4))
RMINC=ABS(P(5))
RMAXC=ABS(P(6))
IF(NP.EQ.6) 6,7
6 HMINI=C(13)
HMAXI=C(14)
HMINN=C(15)
HMAXN=C(16)
HMINC=C(17)
HMAXC=C(18)
GO TO 8
7 HMINI=ABS(P(7))
HMAXI=ABS(P(8))
HMINN=ABS(P(9))
HMAXN=ABS(P(10))
HMINC=ABS(P(11))

HMAXC=ABS(P(12))
8 PORI=C(1)
PORN=C(2)
PORC=C(3)
TAUØ=C(4)
DTAU=C(5)
DDTAU=C(6)
XU=C(7)
CW=C(8)
PPEAK=C(9)
VPOVM=C(10)
RPC=C(11)
RRNEC=C(12)
DERRI=RMAXI-RMINI
DEHHI=HMAXI-HMINI
DELRI=DERRI/15.
DELHI=DEHHI/15.
DERRN=RMAXN-RMINN
DEHNN=HMAXN-HMINN
DELRN=DERRN/15.
DELHN=DEHNN/15.
DERRC=RMAXC-RMINC
DEHHC=HMAXC-HMINC
DELRN=DERRC/15.
DELHC=DEHHC/15.
POR=PORI+PORN+PORC
AAN=3.*PORN/(12.57*DERRN*DEHNN)*.9365
AAI=3.*PORI/(12.57*DERRI*DEHHI)*.9365
AAC=(PORC/(3.14*DERRC*DEHHC))* .9365
DO 13 JH=1,15
DO 12 JR=1,15
XJRM1=JR-1
RØI=RMINI+DELRI*XJRM1
XNUMRI=(AAI/(RØI**3))*DELRI*DELHI
VRØI(JH,JR)=4.19*XNUMRI*(RØI**3)
RØN=RMINN+DELRN*XJRM1
XNUMRN=(AAN/(RØN**3))*DELRN*DELHN

```

FIG.1. P(I) are the parameters, and C(I) are the constants used in GNLS
(variables on left are used in model calculations)

Volume	Pressure	
9.99680E-01	1.00000E+06	P
9.99490E-01	2.00000E+06	
9.98990E-01	5.00000E+06	
9.98000E-01	1.00000E+07	
9.95600E-01	2.00000E+07	
9.93000E-01	3.00000E+07	
9.86900E-01	5.00000E+07	
9.65300E-01	1.00000E+08	
8.87200E-01	2.00000E+08	
8.48800E-01	3.00000E+08	
8.18000E-01	4.00000E+08	
7.92000E-01	5.00000E+08	
7.75500E-01	6.00000E+08	
7.63400E-01	7.00000E+08	
7.54100E-01	8.00000E+08	
7.46100E-01	9.00000E+08	
7.38500E-01	1.00000E+09	
7.31000E-01	1.10000E+09	
7.23600E-01	1.20000E+09	
7.02000E-01	1.50000E+09	
6.82000E-01	1.80000E+09	$P_{\max} = 4.0 \times 10^9$
6.72400E-01	2.00000E+09	
6.65900E-01	2.20000E+09	
6.58300E-01	2.50000E+09	
6.52000E-01	2.80000E+09	
6.47900E-01	3.00000E+09	
6.44300E-01	3.20000E+09	
6.39000E-01	3.50000E+09	
6.35600E-01	3.70000E+09	
6.32200E-01	3.90000E+09	
6.30500E-01	4.00000E+09	$2.0 P_{\max} - P$
6.32200E-01	4.10000E+09	
6.35600E-01	4.30000E+09	
6.39000E-01	4.50000E+09	
6.44300E-01	4.80000E+09	
6.47900E-01	5.00000E+09	
6.51500E-01	5.20000E+09	
6.57300E-01	5.50000E+09	
6.63300E-01	5.80000E+09	
6.67500E-01	6.00000E+09	
6.73000E-01	6.20000E+09	
6.81600E-01	6.50000E+09	
6.92500E-01	6.80000E+09	
7.02700E-01	7.00000E+09	
7.15700E-01	7.20000E+09	
7.30600E-01	7.40000E+09	
7.38700E-01	7.50000E+09	
7.47800E-01	7.60000E+09	
7.58200E-01	7.70000E+09	
7.70500E-01	7.80000E+09	
7.89800E-01	7.90000E+09	
8.02800E-01	7.95000E+09	
8.08000E-01	7.97000E+09	
8.10600E-01	7.98000E+09	
8.13200E-01	7.99000E+09	
8.14500E-01	7.99500E+09	
8.15300E-01	7.99800E+09	
8.15500E-01	7.99900E+09	

FIG.2. Input setup to make double-valued variable (volume) look single-valued to GNLS.

couples and the times of the thermocouple readings are not necessarily the ones calculated in the model. Neither of these problems is very difficult to solve.

For the first because GNLS looks at dependent-independent variable pairs, the problem is solved by simply having n consecutive independent variables the same (this leads to some rather odd looking output as will be seen later). CALCY must generate a corresponding set of n dependent-independent variable pairs for each value of the independent variable. This manner of inputting the data is illustrated in Fig. 3.

The second problem is solved by interpolation of the temperatures calculated in CALCY in radius and time to the desired values. These interpolated values are returned to main as CY(I).

RESULTS

The results of the GNLS calculations* for these models are given in Figs. 4 through 10. In Fig. 4 the volumes calculated by CALCY using the "best guess" starting input parameters are compared to the experimental data. In Fig. 5 the best fit values determined by GNLS are compared. As can be seen from Figs. 4 and 5 GNLS has reduced the sum of squares from 2.84×10^{-2} to 2.00×10^{-3} . Plots of this improvement are shown in Figs. 6 and 7.

In Figs. 8 and 9 the temperatures calculated by GNLS are compared to the experimental temperatures for the starting input parameters and the best fit parameters. Here GNLS has reduced the sum of the squares from 2.265×10 (Fig. 8) to 1.659×10^{-1} (Fig. 9). Plots are shown in Figs. 10 and 11.

Appendix A is a listing for GNLS.

*When a nonlinear fitting routine is used with more than one parameter, the starting parameters are very important since the result is not unique. Physical insight is, in general, helpful in choosing starting parameters. In some cases a starting parameter study may be necessary.

Temperatures
at
radii

2.39000E+01	1.00000E-10	}	Time (1)
2.39000E+01	1.00000E-10		
2.39000E+01	1.00000E-10		
2.39000E+01	1.00000E-10		
2.39000E+01	1.00000E-10		
2.39925E+01	1.20000E+01	}	Time (2)
2.39000E+01	1.20000E+01		
2.39000E+01	1.20000E+01		
2.39000E+01	1.20000E+01		
2.38225E+01	1.20000E+01		
2.39000E+01	1.20000E+01	}	
2.41850E+01	2.40000E+01		
2.39888E+01	2.40000E+01		
2.39000E+01	2.40000E+01		
2.39000E+01	2.40000E+01		
2.38775E+01	2.40000E+01	}	
2.39000E+01	2.40000E+01		
2.52633E+01	5.10000E+01		
2.45700E+01	5.10000E+01		
2.41800E+01	5.10000E+01		
2.40833E+01	5.10000E+01	}	
2.39000E+01	5.10000E+01		
2.39000E+01	5.10000E+01		
2.58550E+01	6.30000E+01		
2.49550E+01	6.30000E+01		
2.44550E+01	6.30000E+01	}	
2.41813E+01	6.30000E+01		
2.39000E+01	6.30000E+01		
2.39000E+01	6.30000E+01		
2.65475E+01	7.50000E+01		
2.54438E+01	7.50000E+01	}	
2.47550E+01	7.50000E+01		
2.43625E+01	7.50000E+01		
2.39775E+01	7.50000E+01		
2.39737E+01	7.50000E+01		
2.73446E+01	8.80000E+01	}	
2.59481E+01	8.80000E+01		
2.51446E+01	8.80000E+01		
2.45654E+01	8.80000E+01		
2.40792E+01	8.80000E+01		
2.40000E+01	8.80000E+01	}	
2.80475E+01	1.00000E+02		
2.64437E+01	1.00000E+02		
2.55400E+01	1.00000E+02		
2.48438E+01	1.00000E+02		
2.41775E+01	1.00000E+02		
2.40738E+01	1.00000E+02	}	Time (n)
2.88400E+01	1.12000E+02		
2.70325E+01	1.12000E+02		
2.59400E+01	1.12000E+02		
2.51438E+01	1.12000E+02		
2.43550E+01	1.12000E+02		
2.41738E+01	1.12000E+02		

FIG.3. Input setup using six identical values for the independent variable (time).

SQ=

2.84095223E-02

LAP= 0

COMPARISON OF INPUT DATA AND CALCULATED RESULTS

STANDARD ERROR OF ESTIMATE=		2.48515253E-02	
INPUT DATA (X)	(Y)	CALC (Y)	(INPUT-CALC)
1.00000E+06	9.99680E-01	9.99939E-01	-2.59424E-04
2.00000E+06	9.99490E-01	9.99881E-01	-3.91190E-04
5.00000E+06	9.98990E-01	9.98099E-01	8.90783E-04
1.00000E+07	9.98000E-01	9.90488E-01	7.51223E-03
2.00000E+07	9.95600E-01	9.74374E-01	2.12263E-02
3.00000E+07	9.93000E-01	9.59586E-01	3.34145E-02
5.00000E+07	9.86900E-01	9.36289E-01	5.06112E-02
1.00000E+08	9.65300E-01	9.08480E-01	5.68199E-02
2.00000E+08	8.87200E-01	8.84753E-01	2.44708E-03
3.00000E+08	8.48800E-01	8.66359E-01	-1.75591E-02
4.00000E+08	8.18000E-01	8.46457E-01	-3.04572E-02
5.00000E+08	7.92000E-01	8.31538E-01	-3.95382E-02
6.00000E+08	7.75500E-01	8.16074E-01	-4.05741E-02
7.00000E+08	7.63400E-01	8.01230E-01	-3.78239E-02
8.00000E+08	7.54100E-01	7.87999E-01	-3.38992E-02
9.00000E+08	7.46100E-01	7.76159E-01	-3.00586E-02
1.00000E+09	7.38500E-01	7.65478E-01	-2.69781E-02
1.10000E+09	7.31000E-01	7.55825E-01	-2.48253E-02
1.20000E+09	7.23600E-01	7.47070E-01	-2.34703E-02
1.50000E+09	7.02000E-01	7.24620E-01	-2.26201E-02
1.80000E+09	6.82000E-01	7.07217E-01	-2.52169E-02
2.00000E+09	6.72400E-01	6.97474E-01	-2.50737E-02
2.20000E+09	6.65900E-01	6.88714E-01	-2.28138E-02
2.50000E+09	6.58300E-01	6.71167E-01	-1.88675E-02
2.80000E+09	6.52000E-01	6.67249E-01	-1.52488E-02
3.00000E+09	6.47900E-01	6.61303E-01	-1.34033E-02
3.20000E+09	6.44300E-01	6.55833E-01	-1.15327E-02
3.50000E+09	6.39000E-01	6.48292E-01	-9.29182E-03
3.70000E+09	6.35600E-01	6.43642E-01	-8.04218E-03
3.90000E+09	6.32200E-01	6.39178E-01	-6.97805E-03
4.00000E+09	6.30500E-01	6.37719E-01	-7.21917E-03
4.10000E+09	6.32200E-01	6.39375E-01	-7.17510E-03
4.30000E+09	6.35600E-01	6.42725E-01	-7.12526E-03
4.50000E+09	6.39000E-01	6.46141E-01	-7.14064E-03
4.80000E+09	6.44300E-01	6.51524E-01	-7.22419E-03
5.00000E+09	6.47900E-01	6.55314E-01	-7.41418E-03
5.20000E+09	6.51500E-01	6.59395E-01	-7.89468E-03
5.50000E+09	6.57300E-01	6.65992E-01	-8.69175E-03
5.80000E+09	6.63300E-01	6.73457E-01	-1.01568E-02
6.00000E+09	6.67500E-01	6.79004E-01	-1.15042E-02
6.20000E+09	6.73000E-01	6.85254E-01	-1.22540E-02
6.50000E+09	6.81600E-01	6.96752E-01	-1.51524E-02
6.80000E+09	6.92500E-01	7.11572E-01	-1.90718E-02
7.00000E+09	7.02700E-01	7.23720E-01	-2.10202E-02
7.20000E+09	7.15700E-01	7.38493E-01	-2.27928E-02
7.40000E+09	7.30600E-01	7.56244E-01	-2.56439E-02
7.50000E+09	7.38700E-01	7.65177E-01	-2.64773E-02
7.60000E+09	7.47800E-01	7.74319E-01	-2.65190E-02
7.70000E+09	7.58200E-01	7.83801E-01	-2.56006E-02
7.80000E+09	7.70500E-01	7.94511E-01	-2.40115E-02
7.90000E+09	7.89800E-01	8.09289E-01	-1.94892E-02
7.95000E+09	8.02800E-01	8.19601E-01	-1.68008E-02
7.97000E+09	8.08000E-01	8.23530E-01	-1.55300E-02
7.98000E+09	8.10600E-01	8.25840E-01	-1.52399E-02
7.99000E+09	8.13200E-01	8.29090E-01	-1.58900E-02
7.99500E+09	8.14500E-01	8.30211E-01	-1.57113E-02
7.99800E+09	8.15300E-01	8.30340E-01	-1.50400E-02
7.99900E+09	8.15500E-01	8.30383E-01	-1.48829E-02
Pressure	Input volume	Calculated volume	

FIG.4. Volume calculation with starting input parameters.

SQ= 2.00485589E-03

LAP= 20

COMPARISON OF INPUT DATA AND CALCULATED RESULTS

STANDARD ERROR OF ESTIMATE=		6.60180459E-03	
INPUT DATA(X)	(Y)	CALC (Y)	(INPUT-CALC)
1.00000E+06	9.99680E-01	9.99939E-01	-2.59424E-04
2.00000E+06	9.99490E-01	9.99881E-01	-3.91190E-04
5.00000E+06	9.98990E-01	9.98658E-01	3.31959E-04
1.00000E+07	9.98000E-01	9.96506E-01	1.49385E-03
2.00000E+07	9.95600E-01	9.93494E-01	2.10636E-03
3.00000E+07	9.93000E-01	9.88945E-01	4.05500E-03
5.00000E+07	9.86900E-01	9.78830E-01	8.06979E-03
1.00000E+08	9.65300E-01	9.47774E-01	1.75261E-02
2.00000E+08	8.87200E-01	8.91398E-01	-4.19755E-03
3.00000E+08	8.48800E-01	8.50863E-01	-2.06320E-03
4.00000E+08	8.18000E-01	8.22461E-01	-4.46129E-03
5.00000E+08	7.92000E-01	8.00907E-01	-8.90653E-03
6.00000E+08	7.75500E-01	7.83571E-01	-8.07074E-03
7.00000E+08	7.63400E-01	7.69127E-01	-5.72676E-03
8.00000E+08	7.54100E-01	7.56929E-01	-2.82942E-03
9.00000E+08	7.46100E-01	7.46255E-01	-1.54670E-04
1.00000E+09	7.38500E-01	7.36875E-01	1.62512E-03
1.10000E+09	7.31000E-01	7.28512E-01	2.48845E-03
1.20000E+09	7.23600E-01	7.21063E-01	2.53657E-03
1.50000E+09	7.02000E-01	7.02035E-01	-3.48733E-05
1.80000E+09	6.82000E-01	6.87316E-01	-5.31624E-03
2.00000E+09	6.72400E-01	6.78994E-01	-6.59361E-03
2.20000E+09	6.65900E-01	6.71514E-01	-5.61402E-03
2.50000E+09	6.58300E-01	6.61574E-01	-3.27364E-03
2.80000E+09	6.52000E-01	6.52917E-01	-9.17318E-04
3.00000E+09	6.47900E-01	6.47794E-01	1.05806E-04
3.20000E+09	6.44300E-01	6.42989E-01	1.31057E-03
3.50000E+09	6.39000E-01	6.36372E-01	2.62757E-03
3.70000E+09	6.35600E-01	6.32286E-01	3.31439E-03
3.90000E+09	6.32200E-01	6.28374E-01	3.82553E-03
4.00000E+09	6.30500E-01	6.27385E-01	3.41484E-03
4.10000E+09	6.32200E-01	6.28551E-01	3.64904E-03
4.30000E+09	6.35600E-01	6.31506E-01	4.09401E-03
4.50000E+09	6.39000E-01	6.34520E-01	4.47985E-03
4.80000E+09	6.44300E-01	6.39231E-01	5.06916E-03
5.00000E+09	6.47900E-01	6.42556E-01	5.34393E-03
5.20000E+09	6.51500E-01	6.46015E-01	5.48467E-03
5.50000E+09	6.57300E-01	6.51645E-01	5.65534E-03
5.80000E+09	6.63300E-01	6.57823E-01	5.47695E-03
6.00000E+09	6.67500E-01	6.62298E-01	5.20239E-03
6.20000E+09	6.73000E-01	6.67212E-01	5.78802E-03
6.50000E+09	6.81600E-01	6.76090E-01	5.50982E-03
6.80000E+09	6.92500E-01	6.87430E-01	5.06990E-03
7.00000E+09	7.02700E-01	6.96693E-01	6.00665E-03
7.20000E+09	7.15700E-01	7.08167E-01	7.53332E-03
7.40000E+09	7.30600E-01	7.23149E-01	7.45139E-03
7.50000E+09	7.38700E-01	7.32679E-01	6.02072E-03
7.60000E+09	7.47800E-01	7.44454E-01	3.34604E-03
7.70000E+09	7.58200E-01	7.59405E-01	-1.20466E-03
7.80000E+09	7.70500E-01	7.79511E-01	-9.01101E-03
7.90000E+09	7.89800E-01	8.01820E-01	-1.20202E-02
7.95000E+09	8.02800E-01	8.12502E-01	-9.70161E-03
7.97000E+09	8.08000E-01	8.16459E-01	-8.45893E-03
7.98000E+09	8.10600E-01	8.18451E-01	-7.85126E-03
7.99000E+09	8.13200E-01	8.20384E-01	-7.13438E-03
7.99500E+09	8.14500E-01	8.22528E-01	-8.02791E-03
7.99800E+09	8.15300E-01	8.23336E-01	-8.00640E-03
7.99900E+09	8.15500E-01	8.23379E-01	-7.87866E-03
Pressure	Input volume	Calculated volume	

FIG.5. Volume calculation with "best" fit parameters determined by GNLS.

FIG.6. Calculated-input fit for starting parameters.

FIG.7. Calculated-input fit for "best" parameters.

SQ= 2.26568960E+01

LAP= 0

COMPARISON OF INPUT DATA AND CALCULATED RESULTS

STANDARD ERROR OF ESTIMATE=		6.53826127E-01		
INPUT DATA(X)	(Y)	CALC (Y)	(INPUT-CALC)	
1.00000E-10	2.39000E+01	2.39000E+01	0.	
1.00000E-10	2.39000E+01	2.39000E+01	0.	
1.00000E-10	2.39000E+01	2.39000E+01	0.	
1.00000E-10	2.39000E+01	2.39000E+01	0.	
1.00000E-10	2.39000E+01	2.39000E+01	0.	
1.00000E-10	2.39000E+01	2.39000E+01	0.	
1.20000E+01	2.39925E+01	2.39355E+01	5.70100E-02	
1.20000E+01	2.39000E+01	2.39024E+01	-2.44267E-03	
1.20000E+01	2.39000E+01	2.39001E+01	-8.76705E-05	
1.20000E+01	2.39000E+01	2.39000E+01	-1.57748E-06	
1.20000E+01	2.38225E+01	2.39000E+01	-7.75000E-02	
1.20000E+01	2.39000E+01	2.39000E+01	0.	
2.40000E+01	2.41850E+01	2.40532E+01	1.31785E-01	
2.40000E+01	2.39888E+01	2.39234E+01	6.54304E-02	
2.40000E+01	2.39000E+01	2.39027E+01	-2.70022E-03	
2.40000E+01	2.39000E+01	2.39002E+01	-2.25422E-04	
2.40000E+01	2.38775E+01	2.39000E+01	-2.25005E-02	
2.40000E+01	2.39000E+01	2.39000E+01	-1.45677E-08	
5.10000E+01	2.52633E+01	2.47032E+01	5.60089E-01	
5.10000E+01	2.45700E+01	2.41139E+01	4.56050E-01	
5.10000E+01	2.41800E+01	2.39500E+01	2.30003E-01	
5.10000E+01	2.40833E+01	2.39102E+01	1.73099E-01	
5.10000E+01	2.39000E+01	2.39003E+01	-2.71087E-04	
5.10000E+01	2.39000E+01	2.39000E+01	-3.50695E-05	
6.30000E+01	2.58550E+01	2.51276E+01	7.27357E-01	
6.30000E+01	2.49550E+01	2.42735E+01	6.81461E-01	
6.30000E+01	2.44550E+01	2.40032E+01	4.51783E-01	
6.30000E+01	2.41813E+01	2.39254E+01	2.55875E-01	
6.30000E+01	2.39000E+01	2.39011E+01	-1.06039E-03	
6.30000E+01	2.39000E+01	2.39002E+01	-1.80304E-04	
7.50000E+01	2.65475E+01	2.56336E+01	9.13926E-01	
7.50000E+01	2.54438E+01	2.44809E+01	9.62929E-01	
7.50000E+01	2.47550E+01	2.40802E+01	6.74815E-01	
7.50000E+01	2.43625E+01	2.39510E+01	4.11464E-01	
7.50000E+01	2.39775E+01	2.39030E+01	7.45131E-02	
7.50000E+01	2.39737E+01	2.39006E+01	7.30822E-02	
8.80000E+01	2.73446E+01	2.62220E+01	1.12259E+00	
8.80000E+01	2.59481E+01	2.47532E+01	1.19491E+00	
8.80000E+01	2.51446E+01	2.41924E+01	9.52212E-01	
8.80000E+01	2.45654E+01	2.39928E+01	5.72646E-01	
8.80000E+01	2.40792E+01	2.39072E+01	1.72022E-01	
8.80000E+01	2.40000E+01	2.39017E+01	9.82507E-02	
1.00000E+02	2.80475E+01	2.67784E+01	1.26912E+00	
1.00000E+02	2.64437E+01	2.50353E+01	1.40844E+00	
1.00000E+02	2.55400E+01	2.43209E+01	1.21914E+00	
1.00000E+02	2.48438E+01	2.40455E+01	7.98313E-01	
1.00000E+02	2.41775E+01	2.39138E+01	2.63709E-01	
1.00000E+02	2.40738E+01	2.39038E+01	1.70011E-01	
1.12000E+02	2.38400E+01	2.73468E+01	1.49318E+00	
1.12000E+02	2.70325E+01	2.53389E+01	1.69360E+00	
1.12000E+02	2.59400E+01	2.44697E+01	1.47031E+00	
1.12000E+02	2.51438E+01	2.41119E+01	1.03191E+00	
1.12000E+02	2.43550E+01	2.39238E+01	4.31215E-01	
1.12000E+02	2.41738E+01	2.39072E+01	2.66586E-01	

Time

Input
temperaturesCalculated
temperatures

FIG.8. Temperature calculation with starting input parameters.

P(1) = 4.66660432E-06
 SQ= 1.65892703E-01

LAP= 14

COMPARISON OF INPUT DATA AND CALCULATED RESULTS

STANDARD ERROR OF ESTIMATE=		5.59468587E-02	
INPUT DATA(X)	(Y)	CALC (Y)	(INPUT-CALC)
1.00000E-10	2.39000E+01	2.39000E+01	0.
1.00000E-10	2.39000E+01	2.39000E+01	0.
1.00000E-10	2.39000E+01	2.39000E+01	0.
1.00000E-10	2.39000E+01	2.39000E+01	0.
1.00000E-10	2.39000E+01	2.39000E+01	0.
1.00000E-10	2.39000E+01	2.39000E+01	0.
1.00000E-10	2.39000E+01	2.39000E+01	0.
1.20000E+01	2.39925E+01	2.40027E+01	-1.01529E-02
1.20000E+01	2.39000E+01	2.39329E+01	-3.29164E-02
1.20000E+01	2.39000E+01	2.39093E+01	-9.27360E-03
1.20000E+01	2.39000E+01	2.39022E+01	-2.23536E-03
1.20000E+01	2.38225E+01	2.39001E+01	-7.75735E-02
1.20000E+01	2.39000E+01	2.39000E+01	-9.74119E-06
2.40000E+01	2.41850E+01	2.42346E+01	-4.95532E-02
2.40000E+01	2.39888E+01	2.40395E+01	-5.07468E-02
2.40000E+01	2.39000E+01	2.39559E+01	-5.53986E-02
2.40000E+01	2.39000E+01	2.39213E+01	-2.13297E-02
2.40000E+01	2.38775E+01	2.39026E+01	-2.50999E-02
2.40000E+01	2.39000E+01	2.39008E+01	-8.24548E-04
5.10000E+01	2.52633E+01	2.52784E+01	-1.51301E-02
5.10000E+01	2.45700E+01	2.46151E+01	-4.51463E-02
5.10000E+01	2.41800E+01	2.42681E+01	-8.80561E-02
5.10000E+01	2.40833E+01	2.40866E+01	-3.25273E-03
5.10000E+01	2.39000E+01	2.39456E+01	-4.55669E-02
5.10000E+01	2.39000E+01	2.39227E+01	-2.27345E-02
6.30000E+01	2.58550E+01	2.59035E+01	-4.85071E-02
6.30000E+01	2.49550E+01	2.49860E+01	-3.09714E-02
6.30000E+01	2.44550E+01	2.44914E+01	-3.63770E-02
6.30000E+01	2.41813E+01	2.42209E+01	-3.96393E-02
6.30000E+01	2.39000E+01	2.39930E+01	-9.29600E-02
6.30000E+01	2.39000E+01	2.39516E+01	-5.15906E-02
7.50000E+01	2.65475E+01	2.65985E+01	-5.10106E-02
7.50000E+01	2.54438E+01	2.54263E+01	1.75248E-02
7.50000E+01	2.47550E+01	2.47688E+01	-1.38189E-02
7.50000E+01	2.43625E+01	2.43947E+01	-3.21697E-02
7.50000E+01	2.39775E+01	2.40617E+01	-8.41591E-02
7.50000E+01	2.39737E+01	2.39972E+01	-2.34749E-02
8.80000E+01	2.73446E+01	2.73480E+01	-3.37775E-03
8.80000E+01	2.59481E+01	2.59349E+01	1.32138E-02
8.80000E+01	2.51446E+01	2.51104E+01	3.42184E-02
8.80000E+01	2.45654E+01	2.46218E+01	-5.63769E-02
8.80000E+01	2.40792E+01	2.41630E+01	-8.38341E-02
8.80000E+01	2.40000E+01	2.40690E+01	-6.90203E-02
1.00000E+02	2.80475E+01	2.80350E+01	1.24575E-02
1.00000E+02	2.64437E+01	2.64144E+01	2.92944E-02
1.00000E+02	2.55400E+01	2.54462E+01	9.38438E-02
1.00000E+02	2.48438E+01	2.48567E+01	-1.28759E-02
1.00000E+02	2.41775E+01	2.42810E+01	-1.03474E-01
1.00000E+02	2.40738E+01	2.41578E+01	-8.39698E-02
1.12000E+02	2.88400E+01	2.87272E+01	1.12789E-01
1.12000E+02	2.70325E+01	2.69050E+01	1.27476E-01
1.12000E+02	2.59400E+01	2.57980E+01	1.41959E-01
1.12000E+02	2.51438E+01	2.51110E+01	3.27592E-02
1.12000E+02	2.43550E+01	2.44206E+01	-6.55935E-02
1.12000E+02	2.41738E+01	2.42680E+01	-9.42477E-02
Time	Input temperatures	Calculated temperatures	

FIG.9. Temperature calculation with best fit parameters determined by GNLS.

FIG.10. Calculated-input fit for starting parameters (quality of fit can be judged from distance between peaks in solid line and top line of data points).

FIG.11. Calculated-input fit for best parameters.

APPENDIX A.

```

$CHAT ((TV80LIB,ORDERLIB,^) FGNLS,GNLS,NLSBINS,NLS,Y88,M,M,L
PROGRAM GNLS(ND,TAPE2=ND,XNR,TAPE3=XNR)
C
C      ++++++ GNLS ++++++      VERSION B
C      CONTENTS : MAIN,EQFIT,LSQ,VIEWCM,CALCY
C
C      CALL CHANGE(7H+NLS77D)
C
C      CLICHE SKINNY
C
C      COMMON /PSTEPS/ VPRI(100), VPRN(100), VPRC(100), D(100)
1      , VOV0(100), X(100,5), Y(100), CY(100)
C
C      COMMON /MATRIX/ VR0I(16,16), VR0N(16,16), VR0C(16,16)
1      , VRR(16,16), VRR1(16,16), VRRN(16,16)
2      , RR(16,16), RR0N(16,16)
3      , VR0IF(31,31), VR0NF(31,31)
C
C      COMMON /MISC/ P(20), C(20), ID(8), TAU, XU, CW, G(5), KP
1      , NDT, NV, RMINI, RMAXI, RMINN, RMAXN, RMINC, RMAXC
2      , HMINI, HMAXI, HMINN, HMAXN, HMINC, HMAXC, PORI, PORN
3      , PORC, PPEAK, VPOVM, AAI, AAN, AAC, DELRI, DELRN, DELRC
4      , DELHI, DELHN, DELHC, POR, VPR0, CNPP, XYZ, NP
5      , VPR0C, VPR0I, VPR0N, TAU0, DTAU, DDTAU, RPC, RRNEC
C
C      ENDCliche
C
C      USE SKINNY
C
C      CALL CREATE(3HXNR,100000,MWD)
C      READ IN DATA
      READ INPUT TAPE 2,1,(ID(J),J=1,8)
40 WRITE OUTPUT TAPE 3,2
      WRITE OUTPUT TAPE 3,1,(ID(J),J=1,8)
      READ INPUT TAPE 2,1
      WRITE OUTPUT TAPE 3,1
      READ INPUT TAPE 2,4,NDT,NV
      WRITE OUTPUT TAPE 3,4,NDT,NV
      IF (NDT) 999,999,42
42 DO 44 J=1,NDT
      READ INPUT TAPE 2,3,Y(J),(X(J,I),I=1,NV)
44 WRITE OUTPUT TAPE 3,6,Y(J),(X(J,I),I=1,NV)
      CALL EQFIT
      GO TO 40
999 CONTINUE
      CALL VIEWCM(1.,1.,1,1.,1,1,ID,1)
      CALL EMPTY(3)
      CALL ASSIGN(3,0,3HXNR,-1)
CC      CALL GIVHSP(3HY88,4HPXNR,IERR)
      CALL EXIT(1)
1      FORMAT(8A10)
2      FORMAT(10H1      INPUT      //)
3      FORMAT(6F12.5)
4      FORMAT(2I6)
5      FORMAT(6(2X,E12.5))
      END
C
* FORTRAN

```



```

WRITE OUTPUT TAPE 3,16
SQB = SQ
GO TO 150
133 LAST = 2
L = 1
135 IF (SQ-SQB) 140,148,148
140 SQB = SQ
LB = L
DO 146 J=1,NP
146 PB(J) = P(J)
148 CALL LSQ(SQ,PS,DP,NP,FLAG)
LC = LC + 1
IF (LC-LCM) 149,149,145
149 IF(FLAG)145,120,145
145 WRITE OUTPUT TAPE 3,8,(J,P(J),J=1,NP)
WRITE OUTPUT TAPE 3,10,SQ,L
IF (NCRT) 110,110,150
150 IF (NV-1) 155,155,156
155 CALL VIEWCM(X,Y,NDT,X,CY,NDT,ID,0)
GO TO 157
156 CALL VIEWCM(CY,Y,NDT,CY,CY,NDT,ID,0)
157 CONTINUE
CALL SETCH (20.,62.,0,0,0,0,0)
WRITE OUTPUT TAPE 100,4,(ID(J),J = 1,8)
CALL SETCH (10.0, 1.0,0,0,0,0,0)
WRITE OUTPUT TAPE 100,13,P(1),P(2),P(3),P(4),P(5),SQ,L
GO TO (133,110,999),LAST
200 CONTINUE
DO 205 J=1,NP
205 P(J) = PB(J)
CALL CALCY
SQ = 0.0
DO 210 J=1,NDT
D(J)=Y(J)-CY(J)
210 SQ=SQ+D(J)**2
WRITE OUTPUT TAPE 3,1
WRITE OUTPUT TAPE 3,4,(ID(J),J=1,8)
WRITE OUTPUT TAPE 3,3
WRITE OUTPUT TAPE 3,8,(J,P(J),J=1,NP)
WRITE OUTPUT TAPE 3,10,SQ,LB
SEE=SQRTF(SQ/DF)
WRITE OUTPUT TAPE 3,12,SEE
WRITE OUTPUT TAPE 3,11,(X(J,1),Y(J),CY(J),D(J),J=1,NDT)
L = LB
LAST = 3
GO TO 150
900 WRITE OUTPUT TAPE 3,19,L
WRITE OUTPUT TAPE 3,8,(J,P(J),J=1,NP)
999 CONTINUE
RETURN
1 FORMAT(1H1)
2 FORMAT (1H1,10X,40H CALCULATIONS WITH ORIGINAL PARAMETERS ///)
3 FORMAT (/// 15X,32H RESULTS FOR BEST PARAMETERS. ///)
4 FORMAT(1H, 8A10)
5 FORMAT (2F12.6,4I6)
6 FORMAT (3I6)
7 FORMAT(6F12.3)
8 FORMAT( 3H P(I2, 4H) = E20.8)
10 FORMAT (4H SQ=E20.8,10X,5H LAP=I4 ///)
11 FORMAT(26H INPUT DATA(X) (Y),14X,8H CALC (Y),11X,12H INPUT-

```

```

1CALC) /( 1P2E15.5,2E20.5))
12 FORMAT(48H COMPARISON OF INPUT DATA AND CALCULATED RESULTS//
128H STANDARD ERROR OF ESTIMATE= E20.8)
13 FORMAT ( 6H1INPUT,10X,3HNO.,13,4H OF,13,18H PARAMETER SETS
1 ,//5X ,8A10// 10X,21G,2F12.6,41G//)
15 FORMAT (3H C(12,4H) = E20.8)
16 FORMAT (11H1ITERATIONS ///)
17 FORMAT ( // )
18 FORMAT (5E14.5,E20.4, 10H LAP = ,15)
19 FORMAT (45H OVERTFLOW ERROR IN CY(J) CALCULATION AT LAP = ,14/
1 23H CURRENT PARAMETERS ARE )
END

```

```

C
C
* FORTRAN
SUBROUTINE LSQ(SQ,P,DP,N,FLAG)
DIMENSION P(1)
L = L
J = J
IF (FLAG) 50,57,55
50 L = 1
DLTP = DP
51 FLAG = 0.0
J = 1
DMAX = 0.0
SSQ1 = SQ
53 P(J) = P(J)+DLTP
NB = 53
GO TO 999
55 L = 2
GO TO 51
57 GO TO(60,60,85,85),L
60 P(J) = P(J)-DLTP
U = SQ-SSQ1
IF(ABSF(U)-DMAX)65,65,62
62 DMAX = ABSF(U)
65 KJ = J + 2*N
P(KJ) = U
J = J+1
IF (N-J) 68,53,53
68 IF (DMAX) 69,69,70
69 J = 1
DLTP = 2.0*DLTP
GO TO 53
70 GO TO(72,77,77,77),L
72 DO 75 I=1,N
K = I+N
KK = I+2*N
75 P(K) = P(KK)/DMAX
KTR = 1
L = 4
GO TO 88
77 C = DLTP/DMAX
DO 80 I=1,N
KK = I+2*N
U = P(I)+C*P(KK)
P(KK) = P(I)
80 P(I) = U
KTR = 2
L = 3

```

```

      NB = 80
      GO TO 999
85   KTR = KTR-1
      IF(KTR) 95,92,87
87   SSQ1 = SQ
88   DO 90 I=1,N
      K = I+N
90   P(I) = P(I)+DLTP*P(K)
      NB = 90
      GO TO 999
92   SSQ2 = SQ
      GO TO 88
95   DEN = 2.0*(SQ-2.0*SSQ2+SSQ1)
      IF( ABSF(DEN)-SQ*1.0E-7)100,100,102
100  DLTP = 2.0*DLTP
      KTR = 0
      GO TO 92
102  IF (DEN)103,104,104
103  DEN = -2.0 * DEN
104  DTMIN = (4.0*SSQ2-3.0*SQ-SSQ1)/DEN
      IF(ABSF(DTMIN)-50.0) 107,105,105
105  DTMIN = SIGNF(50.0,DTMIN)
      KTR = 2
      GO TO 112
107  GO TO(110,110,112,110),L
110  IF(ABSF(DTMIN+2.0)-4.0) 111,111,112
111  DLTP = DLTP/2.0
      DTMIN = DTMIN*2.0
112  U = DTMIN*DLTP
      DO 115 I=1,N
      K = I+N
115  P(I) = P(I) + U*P(K)
      IF (KTR - 2) 116,130,116
116  GO TO(120,120,120,117),L
117  FLAG = 1.0
      NB = 117
      GO TO 999
120  DMAX = 0.0
      DO 122 I=1,N
      K = I+N
      KK = I+2*N
      U = P(KK) - P(I)
      IF (ABSF(U) - DMAX) 122,121,121
121  DMAX = ABSF(U)
122  P(K) = U
      DO 125 I=1,N
      K = I+N
125  P(K) = P(K)/DMAX
      L = 4
      KTR = 2
130  NB = 130
999  CONTINUE
      RETURN
      END
C
C
*  FORTRAN
      SUBROUTINE VIEWCM (X1,Y1,N1,X2,Y2,N2,DDID,NEND)
C      DDID(1) = 6HBOX199      DDID(2) = 6H-----      NEND = 0      TILL L
      DIMENSION XMI(4),YMI(4),X1(1),X2(1),Y1(1),Y2(1)      ,DDID(1)

```



```

      IF(NEND) 10,10,12
12  IFRST=0
      CALL PLOTE
33  VRR(J,I) = TEMP+TVRR
10  IF (IFRST) 14,14,16
14  IFRST = 1
      CALL CRTID(6HNLS77D,1,1,DDID)
CC
      CALL KEEPE0(1)
CC
16  CONTINUE
      CALL CARTMM (N1,XMI(1),XMI(2),X1,1)
      CALL CARTMM (N1,YMI(1),YMI(2),Y1,1)
      CALL CARTMM (N2,XMI(3),XMI(4),X2,1)
      CALL CARTMM (N2,YMI(3),YMI(4),Y2,1)
      CALL CARTMM (4,XMIN,XMAX,XMI,1)
      CALL CARTMM (4,YMIN,YMAX,YMI,1)
      CALL FRAME(1)
      CALL MAPG(XMIN,XMAX,YMIN,YMAX)
      CALL SETPCH(0,0,0,0,12)
      CALL POINTC(1H+,X1,Y1,N1,1,1)
      CALL TRACE(X2,Y2,N2,1,1)
      RETURN
      END
C
*  FORTRAN
      SUBROUTINE CALCY
C
C
C
      USE SKINNY
      MODEL
      RETURN
      END

```

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