BURSUB AND DEPOR VERSION 3.50 - TWO FORTRAN 77 PROGRAMS FOR POROSITY AND SUBSIDENCE ANALYSIS

F.M.Gradstein*, J.M.Fearon and Z. Huang**

* Atlantic Geoscience Centre
Bedford Institute of Oceanography
Dartmouth, Nova Scotia, B2Y 4A2

** Department of Geology
Dalhousie University
Halifax, Nova Scotia, B3H 3J5

Geological Survey of Canada - Open File no 1283 (1989)

Geological Survey of Canada
601 Booth Street
Ottawa, Ontario, K1A OE8

Note: BURSUB and DEPOR VERSION 3.50 - release date 31 July 1989 replaces BURSUB and DEPOR VERSION 3.00, Geological Survey of Canada Open File 1283, issued 31 January 1989.

DEPOR AND BURSUB VERSION 3.50

The PC based F77 program DEPOR calculates decompaction parameters from porosity-depth trends; the companion program BURSUB calculates sedimentation, burial and subsidence trends. Both programs operate on stratigraphic well data in single sites.

Using BURSUB, a well is divided into time-successive units whose age in Ma, depth, minimum and maximum paleo water depth, minimum and maximum eustatic sea level height, lithology, decompaction function, and decompaction parameters (the latter from DEPOR) are specified. The history of the well site is reconstructed from calculation of sedimentation, burial and subsidence rates and depths below sea level through time for "basement" and successive age levels. For details of these computations, see Stam et al. (1987).

The program features of VERSION 3.50 are extensive and are listed below.

1. DEPOR 3.50 calculates decompaction parameters from depth-porosity data files with up to 500 levels, using linear-, exponential-, "power law"-, reciprocal, and parabolic best fit functions.

2. BURSUB 3.50 has built-in decompaction default values for 8 common lithologies, based on global data sets, with emphasis on shales.

3. For both programs there is a standard parameter (input) file, outside the main program that defines

   a) physical constants,
   b) 20 or more lithology types and its associated decompaction functions,
   c) grain densities, and
   d) DOS 3.2 , Printer and Plotter instructions.

4. The stratigraphic data input file for BURSUB 3.50 has been enhanced and expanded; it allows 100 stratigraphic horizons per well site. Disconformities where age increases but not depth must be simulated with a minimal increase of depth (e.g. 1 m). If decompaction functions and/or grain densities per lithology are defined in the data input file, than the program ignores defaults for these parameters as built-in the parameter file.

5. There is a conversion program for change of files with stratigraphic data input format from Version 2 to Version 3.50.

6. BURSUB 3.50 has extensive, new graphics of results. A central display menu allows the user to select one of ten different plots featuring:

   a) Burial Curves
   b) Paleo waterdepth and sealevel
   c) Tectonic subsidence 1
   d) Tectonic Subsidence 2
   e) Decompacted Burial Curves for all age levels
   f) Restored Sedimentation Rates
   g) Uncorrected Burial Rates
   h) Decompacted Burial Rates
   i) Subsidence Rates

   Plots a-e are cumulative trends; plots f-i are bargraphs. Plot scales can be adapted as needed, and are defined by the user in the data input file.

7. Both DEPOR and BURSUB feature extensive HELP MENUS and HELP FILES, that may be called during execution.

8. ASCII Readme1.doc and Readme2.doc files explain the content of the two 5 1/4 floppy disks (numbers 1 and 2) on which the programs are issued.

9. The original Profort F77 source code of Version 2 has been rewritten for Lahey FORTRAN 77 (F77L) version 2.22, which significantly enhances the use of F77 and allows distribution of execution modules; it also allows to interrupt program execution for calls to DOS. The graphics now makes use of the Graphics Development Toolkit Version 2.12, produced by Graphics Software Systems (GSS), that allows utilization of a wide range of display, plotter and printer device.

10. The programs structure is now completely modular with common areas and subprograms for separate numerical and graphics versions of BURSUB. Storage of all program variables is in common blocks for simple program modifications.

References

Stam, B., Gradstein, F.M., Lloyd, P. and Gillis, D., 1987. Algorithms for porosity and subsidence history. Computers and Geoscience, 13,(4),317-349.

Interpretation of results with DEPOR and BURSUB

The calculation of sedimentation, burial and subsidence rates and their cumulative trends through time, has essentially not been modified from BURSUB version 3.00 to BURSUB version 3.50. Thus, for the methodology and explanation of results with BURSUB 3.50, the reader is referred to Stam et al. (1987).

On the other hand, DEPOR version 3.50 has been modified in that it can fit depth-porosity data using a parabolic function. DEPOR version 3.50 deals with the detailed calculation and testing of the best possible linear or curvilinear fit of porosity-depth data for each lithological type in a well site. Below is a brief explanation of the method and terminology encountered in output using this program.

Best fits are applied to the porosity-depth data for each lithological type. The porosities are the dependent variable.

The fit of all default functions defined for the lithological type in the parameter file is considered first. (A function type will be omitted here when the parameter file has no default for that function type.) The first function tested is the "null" function, $\varnothing = 0$, because any function with a fit worse than this would of course be rejected out of hand. DEPOR reports the residual SOS for each. "Residual SOS" is the residual sum of squares of the observed porosities from the values predicted by an equation, $\varnothing(z)$:

$$\sum \left[y_i - \varnothing(z_i)\right]^z$$

Since no parameters are estimated for these functions, the residual SOS has n degrees of freedom, where n is the number of observed porosities for the lithological type.

Function of each type (0-5; see below and Figure 1) are then fitted to the data. The first is the constant function, $\varnothing = y$, where y is the mean porosity for the lithological type: any default function used in BURSUB should fit at least as well as this, and any fitted function used in BURSUB should be significantly better. Since mean porosity is estimated from the data, the residual SOS for this function has $n - 1$ degrees of freedom.

If the best default function fits better than mean porosity, then it is adopted as the standard against which the other fitted functions will be compared; otherwise mean porosity is adopted as the standard. DEPOR reports the outcome of this comparison.

The function types 1, 2, 3 or 4 (Figure 1) estimate two parameters from the data (α and β) and function type 5 (Figure 1) estimates three parameters from the data (α, β,γ); consequently they must all fit the data better than mean porosity, and their residual SOS has only $n - 2$ two degrees of freedom. (A function type is omitted by DEPOR if the least squares procedure yields an "illegal" depth-porosity function, e.g. when $\varnothing(z) > 1$ for some z or when it is increasing instead of decreasing downhole.) DEPOR reports the residual SOS for each and states which of them gives the best fit.

The "benefit" obtained from using the best of the fitted functions is the amount by which its residual SOS is less than that of the standard of comparison; the "cost" of using it is the additional degree(s) of freedom absorbed in estimating the parameters. This function should not be used unless the "benefit" outweighs the "cost"; i.e. unless the reduction in residual SOS is *significant*.

When a default function is the standard of comparison, the variance attributable to the fitted function is the reduction in residual SOS divided by the two degrees of freedom absorbed in estimating the parameters; when mean porosity is the standard, the reduction in residual SOS is divided by the one degree of freedom absorbed in estimating the extra *second* parameter. The "error" variance is estimated by dividing the residual SOS for the fitted function be $n - 2$, its degrees of freedom. If Fisher's F, the ratio of these variances, is not significant, then the reduction in residual SOS for the fitted function is no better than could be expected by chance; in that case the "cost" outweighs the "benefit", and the standard should be used for BURSUB in preference to the best fitted function.

The function types (Figure 1) are as follows:

Type 0: A constant function, $\varnothing = \alpha$
Type 1: A linear function, $\varnothing = \alpha - \beta z$
Type 2: An exponential function, $\varnothing = \alpha . e^{-\beta z}$.
Type 3: A "power-law" function, $\varnothing = 1 - \alpha z^{\beta}$.
Type 4: A reciprocal function, $\varnothing = 1/(\alpha + \beta z)$.
Type 5: A parabolic function, $\varnothing = \alpha z^2 + \beta z + \gamma$

For function types 2-4, the data are transformed to reduce the function to a linear form and the parameters are estimated by the method of weighted least squares.

Types 0 and 1 are already linear and do not need transformation; for the remainder, the linear form is:

Type 2: $ln(\varnothing) = ln(\alpha) - \beta z$
Type 3: $ln(1-\varnothing) = ln(\alpha) - \beta ln(z)$.
Type 4: $1/\varnothing = \alpha + \beta z$.

Let y be observed porosity and let y' be its transformed value (e.g. $y' = 1n[1-y]$ for type 3). The method of ordinary least squares minimizes the squared deviations of y' from the corresponding linear form of the equation; but it does not follow that the squared deviations of y itself from the untransformed function will be minimized. In order to improve the fit for y itself, the squared deviations of y' from the linear form are multiplied by weights, $w = [dy/dy']^2$ (see Kempthorne, 1967). The weights used with the transformed functions are:

Type 2: $w = y^2$
Type 3: $w = (1-y)^2$
Type 4: $w = y^4$

More detailed methods of achieving the same are given by Bard (1974).

The equations for linear and "power-law" functions may yield *calculated* porosities less than zero. BURSUB treats these as "piece-wise" functions, and calculates a porosity of zero in such cases. DEPOR, however, does not include these "piece-wise" functions among the candidates over which the residual SOS is minimized. Fitted functions which yield a negative porosity at the largest depth in the data should be treated with caution. (See documentation of depth-porosity function types in BURSUB for details.)

For function type 5, the data are also transformed to reduce the function to a linear form. The parameters (α, β and γ) are calculated by least squares on the basis of a High Speed Matric Generator (HSMG) (Thompson, G.T. et al., 1988). Therefore, no weight is used.

Function type 5 fitted must be a decreasing function in the depth range of the data concerned. If the minimum of this function is in the depth range of the data concerned, this function is discarded.

For the runs test in DEPOR version 3.50, an observed porosity is considered a " + " if $y_i \geq \varnothing(z_i)$ and a " - " if $y_i < \varnothing(z_i)$. This is done for the whole well section, using the best of the fitted equations for the lithological type at z_i. The plusses and minuses are arranged in a sequence corresponding to increasing values of z_i. The "total number of runs" is the number of times a plus is followed by a minus, or *vice versa*, in this sequence. The "number of cases above predicted value" is the number of plusses in the sequence; the "number of cases below predicted value" is the number of minuses.

If the fitted curves have regions in the well section where they tend to be *systematically* above or below the data, the total number of runs will be fewer than could be expected by chance. On the other hand, if the data tend to be cyclic, there will be more runs than expected. This is therefore a standard test for the adequacy of a fitted function, and is described in standard textbooks on non-parametric statistics. If the total number of runs is significantly different from the expected number, the graph of the data and the fitted functions should be examined carefully to determine where the problem lies and whether the fitted functions (or the data) are acceptable.

The "expected number" is the mean number of runs expected in a random sequence of plusses and minuses; the "standard deviation" is the standard deviation of this mean in a random sequence. The "normal deviate" is the difference between the observed number of runs and the expected number divided by the standard deviation; this may be looked up in tables of the normal distribution in statistical textbooks. If the number of plusses and the number of minuses are both less than 20, then the significance of the observed number must be looked up in a table which will be found in texts on non-parametric statistics, for example Section 11.2 and Table IX in Bradley (1968).

References

Bard, Y. 1974. Nonlinear parameter estimation. Academic Press.

Bradley, J.V. 1968. Distribution-free statistical tests. Prentice-Hall.

Kempthorne, O. 1967. Design and analysis of experiments. Wiley.

Stam,B., Gradstein,F.M., Lloyd,P. and Gillis,D. 1987. Algorithms for porosity and subsidence history. Computers and Geoscience, 13,(4),317-349.

Thompson, G,T, and Balch, S.J. 1988. An efficient algorithm for polynomial curve fitting. Computers and Geoscience, 14,(5),547-556.

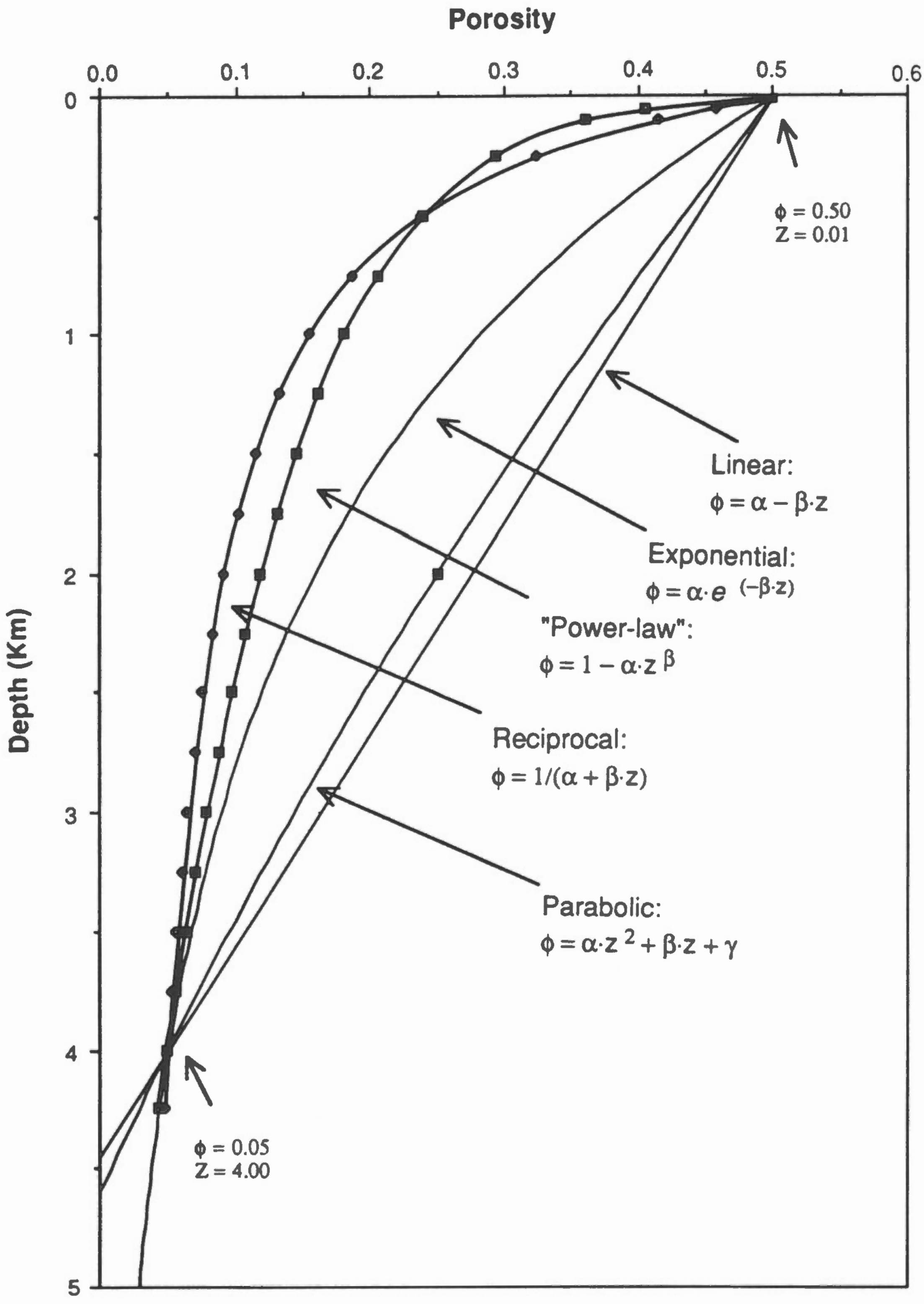

Figure 1. Comparison of depth-porosity function types. For the purpose of this example, each function is required to pass through two fixed points, as shown.

CONTENTS OF DISKETTE 1 (5.25")

ASCII FILE README1.DOC

NOTE: Some files contain ASCII characters above 127 (dec.) which will display correctly on a monitor but may not reproduce correctly on a non-graphics printer.

This diskette contains the F77 load modules of Version 3.50 for the programs BURSUB, DEPOR and RUNCONV. These programs execute on IBM-PCXT micro-computer with 8087 math co-processor. Details on installation of the graphics version of BURSUB are below and on diskette 2. Several data input files are included. In the root directory of this diskette you will find:

1. README1.DOC - this file.

2. OF1283.DOC - File that describes new features in BURSUB and DEPOR VERSION 3.50, released as Geological Survey of Canada Open File 1283, 1989.

Sub-directory BURSUB contains:

1. BURSUB.EXE - Load module of BURSUB 3.50 without graphics. The program requires a minumum of 153 KB of free memory. A mathematical co-processor is required. The program can be compiled with graphics when GSS Graphics Development Toolkit (version 2.12) has been installed (see diskette 2); in that case 350 KB of free memory will be required; ANSI.SYS, the DOS driver for the monitor, must be invoked by the following line in the CONFIG.SYS file:
   DEVICE = [path]ANSI.SYS

2. BURSUB.PAR - Standard parameter file both with BURSUB and with DEPOR VERSION 3.50. It contains:

   a) default parameters on physical constants,
   b) lithology types and their input codes for the data input files to BURSUB and DEPOR,
   c) grain density values,
   d) parameter values for default depth/porosity functions and their codes for the data input files for BURSUB and DEPOR,
   e) DOS 3.2 and plot and printer instructions.

   BURSUB.PAR can be modified as required, without recompilation of the main program.

3. BURSUB.HLP - help file; may be invoked during execution of BURSUB.

4. MURRE.SUB - data input file for BURSUB 3.50, using the Murre well, Grand Banks; this file has input instructions.

5. MURRE.OUT - results, using BURSUB 3.50 on MURRE.SUB.

6. VIGO.SUB - data input file for BURSUB 3.50, using DSDP Site 398, Vigo Seamount.

Sub-directoy DEPOR contains:

1. DEPOR.EXE - Load module of DEPOR 3.50. The program requires 106 KB of free memory. A mathematical co-processor is required. The parameter file for DEPOR is BURSUB.PAR in sub-directory BURSUB. DEPOR, like BURSUB, requires that ANSI.SYS be invoked by the CONFIG.SYS file.

2. DEPOR.HLP - help file; may be invoked during execution of DEPOR.

3. VIGO1.DEP - depth/lithology file for DSDP Site 398, Vigo Seamount; uses BURSUB.PAR for execution with DEPOR.

4. VIGO2.DEP - depth/porosity file for DSDP Site 398, Vigo Seamount.

5. X1.DEP - depth/lithology file for Site X.

6. X2.DEP - depth/porosity file for Site X.

7. X.PAR - Parameter file for execution of X1.DEP and X2.DEP.

8. X.OUT - Results using DEPOR on X1.DEP and X2.DEP.

Sub-directory RUNCONV contains:

1. RUNCONV.EXE - Program to convert run files for earlier versions of BURSUB (elder than version 3.00) to the new format.

2. LITHTYPE.NEW - Data file for RUNCONV specifying the new codes for the lithological types used in earlier versions (older than version 3.00) of the programs.

---

25 July 1989

F.M. Gradstein, M. Fearon and Z. Huang
Atlantic Geoscience Centre
Bedford Institute of Oceanography
Dartmouth, Nova Scotia, B2Y 4A2
Canada

BITNET: GRADSTEI@DALAC

CONTENTS OF DISKETTE 2 (5.25")

ASCII FILE README2.DOC

NOTE: Some files contain ASCII characters above 127 (dec.) which will display correctly on a monitor but may not reproduce correctly on a non-graphics printer.

This diskette contains the FORTRAN source code of Version 3.50 for the programs BURSUB, DEPOR and RUNCONV. Files with the extension FOR are to be compiled. Files with the extension CMN are common areas which are required to satisfy the INCLUDE statement of FORTRAN during compilation. Each file contains one common area or sub-program. The source code was written for compilation by Lahey FORTRAN 77 (F77L) version 2.22. The root directory contains the following:

1. BURSUB.FOR - Source code for the main program of BURSUB version 3.50 (25 July 1989). It requires the CMN files in sub-directory BURSUB.
2. DEPOR.FOR - Source code for the main program of DEPOR version 3.50 (5 June 1989). It requires the CMN files in sub-directory DEPOR.
3. RUNCONV.FOR - Source code for program RUNCONV.
4. README2.DOC - This file.

Sub-directory BURSUB contains the common areas and sub-programs required by both the numerical and the graphics version of program BURSUB. The following files are included:

1. BURINF01.CMN	2. IOFIL00.CMN	3. BURINI00.FOR
4. BURTAB01.FOR	5. DECOMP02.FOR	6. DEPDAT01.FOR
7. DIFDAT01.FOR	8. PARCOM02.FOR	9. RDDATA02.FOR
10. RDHLPB00.FOR	11. RDPARB01.FOR	

Sub-directory DEPOR contains the common areas and sub-programs required by program DEPOR. The following files are included:

1. DEPINF01.CMN	2. IOFIL00.CMN	3. DEPINI00 FOR
4. FINDLT01.FOR	5. FITOUT01.FOR	6. FPCHK01.FOR
7. RDHLPD01.FOR	8. RDLITH02.FOR	9. RDPARD01.FOR
10. READDP02.FOR	11. WLSLIN01.FOR	

Sub-directory GRAPHICS contains the common areas and sub-programs required only by the graphics version of program BURSUB. Subroutines BURPLT02 and SELPLT01 will require the CMN files in sub-directory BURSUB as well as those in GRAPHICS. These sub-programs must be linked with version 2.12 of the Graphics Development Toolkit produced by Graphics Software Systems. To eliminate graphics from BURSUB, delete from BURSUB.FOR all lines having the code "@@PLOT@@" in columns 72-80. The following files are included:

1. GRACTL00.CMN	2. POLYGN00.CMN	3. TVALUE00.CMN
4. BURPLT02.FOR	5. CHARAD01.FOR	6. CTSOLV01.FOR
7. CTXSET01.FOR	8. DEVBGN02.FOR	9. GRAINP01.FOR
10. GRID01.FOR	11. GTXSET01.FOR	12. HISTOG01.FOR
13. LINSET02.FOR	14. MRKSET01.FOR	15. RMSKLN00.FOR
16. RMSKPT00.FOR	17. SELPLT01.FOR	

Sub-directory UTILITY contains minor sub-programs required by both BURSUB and DEPOR. The following files are included:

1. ASKA02.FOR	2. CASE01.FOR	3. CEIL.FOR
4. CHOICE00.FOR	5. DOCOUT.FOR	6. DOSCMD00.FOR
7. DPFUNC01.FOR	8. FLOOR.FOR	

Suppliers of Lahey FORTRAN and the Graphics Development Toolkit are:

Lahey Computer Systems,Inc.
P.O. Box 6091
Incline Village
NV 89450-6091
USA
702-831-2500

Graphics Software Systems,Inc.
9590 SW Gemini Dr.
Beaverton
OR 97005
USA

---

25 July 1989

F.M. Gradstein, M. Fearon and Z. Huang
Atlantic Geoscience Centre
Bedford Institute of Oceanography
Dartmouth, Nova Scotia, B2Y 4A2
Canada

BITNET: GRADSTEI@DALAC
