BURSUB AND DEPOR VERSION 3.00 - TWO FORTRAN 77 PROGRAMS FOR POROSITY AND SUBSIDENCE ANALYSIS

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[superseded]

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Note: BURSUB and DEPOR VERSION 3.00 - release data 31 January 1989 replaces BURSUB and DEPOR VERSION 2.01, Geological Survey of Canada Open File 1283, originally issued in December 1986.

DEPOR AND BURSUB VERSION 3.00

The PC based F77 programs DEPOR and BURSUB calculate decompaction parameters and sedimentation, burial and subsidence trends in single well sites.

New program features in VERSION 3.00 are extensive and are listed below.

1. DEPOR 3.00 calculates decompaction parameters from depth- porosity data files with up to 500 levels, using linear-, exponential-, "power law"-, and reciprocal best fit functions.

2. BURSUB 3.00 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 now 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 3.00 has been enhanced and expanded; it allows 100 stratigraphic horizons per well site, with disconformities permitted. If decompaction functions and 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 3.00.

6. BURSUB 3.00 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 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.

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 2 to BURSUB version 3. Thus, for the methodology and explanation of results with BURSUB 3.00, the reader is referred to Stam et al. (1987).

On the other hand, DEPOR version 3.00 has been extensively modified. The conversion of sonic log data in a well to porosity values has been dropped, pending extensive modifications to the basic technique of conversion. It may be released at a later date. DEPOR version 3.00 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 new 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, $\varnothing(z)$:

$$\sum \left[y_i - \varnothing(z_i)\right]^2$$

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 (0-4; 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 other fitted functions all estimate two parameters from the data (α and β); 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.

For each function type, the data are transformed to reduce the function to a linear form and the parameters are estimated by the method of weighted least squares. The function types (Figure 1) are as follows:

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

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

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

Let y be observed porosity and let y' be its transformed value (e.g. $y' = ln[1-y]$ 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 the runs test in DEPOR version 3.00, an observed porosity is considered a " + " if $y_i \geq \emptyset(z_i)$ and a " - " if $y_i < \emptyset(z_i)$. 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. Comp.& Geosc., 13,(4),317-349.

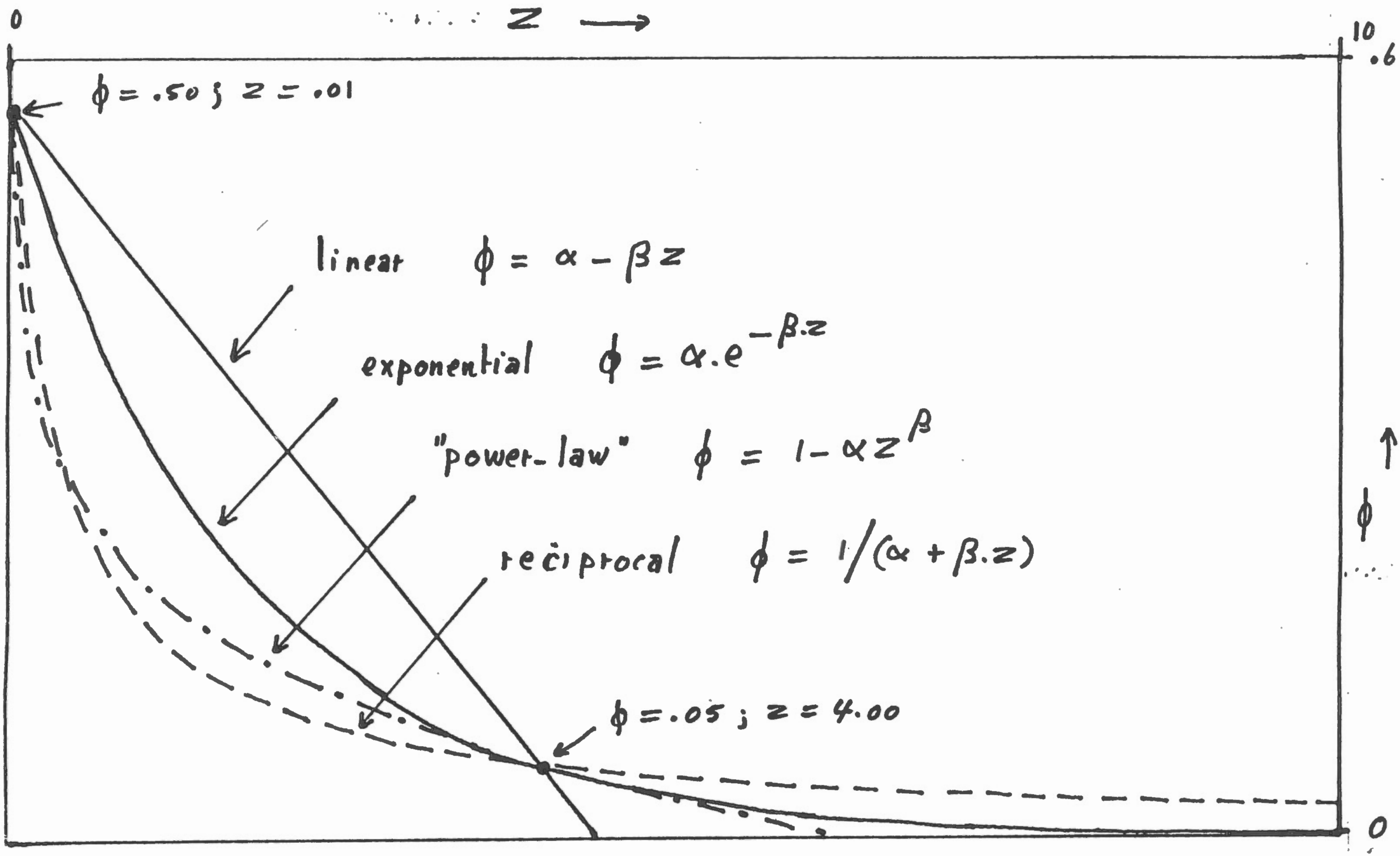

Figure 1. Comparison of depth-porosity function types. For the purpose of this example, each function is required to pass through two fixed points, as shown.