# Introduction

NMR relaxation data and many other kinds of decay data may consist of exponentially decaying components with a small number of discrete relaxation times, or time constants, or there may be a continuous or quasi-continuous distribution of relaxation times over some range. These distributions can be well represented by amplitudes computed from the relaxation data for a predetermined sequence of systematically-spaced relaxation times, usually equally spaced in log-time. However, such computed distributions can contain far more detail than is actually determined by the data, which are always subject to some "noise". The computed distributions are therefore subjected to some kind of smoothing, or "regulation" to avoid detail that is not meaningful.

Uniform PENalty inversion of multiexponential decay data. The name refers to the application of negative feedback to a smoothing "penalty" function to prevent excessive detail in distributions of relaxation times. This allows appropriate smoothing of both sharp peaks and broad features in the same distribution, allowing the sharp peaks without breaking broad features into multiple peaks not required by the data. This allows meaningful computation of the *rms* noise and supports additional UPEN objectives, which include identifying various data features and data problems (such as data not precisely fitting the model of multiexponential decay plus random noise), giving a series of diagnostics and warnings and allowing processing options where needed.
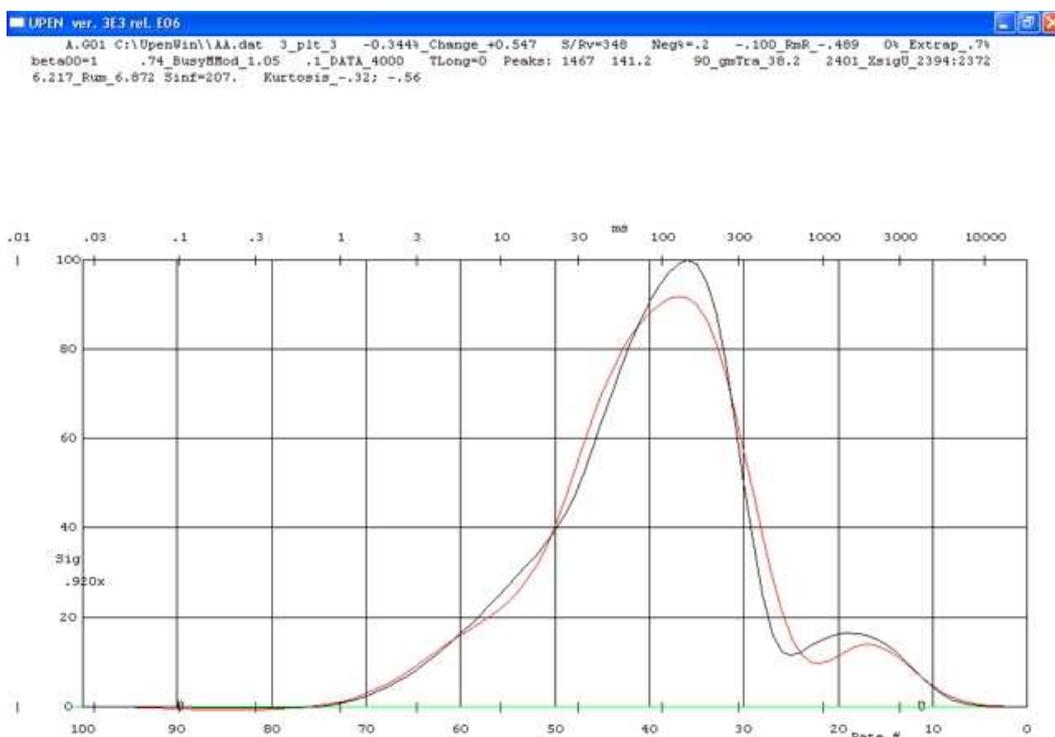
There are many adjustable parameters in UPEN, most of which need not and should not be adjusted except in specialized circumstances or in basic investigation of UPEN function. See under "**Parameters_ Most-Frequently-Adjusted**," "**Parameters_ Less-Frequently-Adjusted**," and "**Parameters_ Seldom- Adjusted**". Parameters referred to will be in the first of these categories unless specified otherwise. Parameters may be adjusted by clicking "Upen Parameters" and selecting one of these three categories or "Restore defaults". Initial values of most parameters can be set also in the initial parameter file, by clicking "par" and proceeding to the desired parameter file (such as Upenpar.par), making any needed changes, and saving or not saving as desired. In addition, a number of parameters can be changed during computation. See the section "**Keyboard Input**".

The input data file for UPEN is a binary file produced by any of several preprocessing "Filters". See "**Input Data File**s" and "Tutorial".

UPEN is an iterative inversion computation, and the evolving distributions and various computed quantities are shown at each iteration. The user can press "p" or "P" to pause. When computation is complete, two text files are produced. A file with the extension .tst lists a number of computed parameters, including some diagnostic quantities. A file with the extension .dat lists the computed distributions in several forms and also lists the data. See "**Output and Display**".

Some miscellaneous Help topics are under **Misc**.

The background and basic algorithm for UPEN, including diagnostic features, is given in two published articles, an article (to be referred to as **UPEN-I**) **Uniform-Penalty Inversion of Multiexponential Decay Data** by Borgia, Brown, and Fantazzini, *Journal of Magnetic Resonance*, **132**, 65-77 (1998) and a second article (to be referred to as **UPEN-II**), **Uniform-Penalty Inversion of Multiexponential Decay Data II. Data Spacing, T_2 Data, Systematic Data Errors, and Diagnostics,** *Journal of Magnetic Resonance* **147**, 273-285 (2000). Another paper is **Examples of Marginal Resolution of NMR Relaxation Peaks Using UPEN and Diagnostics,** *Magnetic Resonance Imaging*, **19**, 473-475 (2001). Reprints or .pdf files are available from the authors.

Windows Interface

UpenWin is a 32 bit application for Windows (currently tested under windows 98, XP and Vista), developed in C++ and MFC (Microsoft Foundation Class) by means of Visual Studio 2005, that implements an interface to facilitate the use of UPEN (Uniform PENalty) and its related input files.

It is composed of a simple SDI (Single Document Interface) application with many dialog boxes. Among other things, it is a simple text editor (window-editor interface) where one can edit the parameters file used for Upen processing. By means of the dialogs the user can pre-process the data file using the appropriate filter program, sets the value for the parameters for UPEN and runs a computation session.

Parameters can be set also in the initial parameter file, by clicking the "par" menu button and proceeding to the desired parameter file (such as Upenpar.par), making any needed changes, and saving or not saving as desired.

When the window-editor interface is empty (no parameters file is loaded) and the user runs a computation session, Upen will use the values of parameters that are set in parameters-dialogs. On the contrary, when a set of parameters is open in the window-editor interface and the user runs a process session, Upen will use the values of parameters shown (on the screen) in the window-editor interface bypassing the values that are set in parameters-dialogs.

Menu System description

File

New: this command creates a document containing a default set of parameters for Upen (parameters sheet) with the default name "Untitled".

Open: this command displays the *Open* dialog box with the default file search extension "*.PAR". Use this command to open an existing parameters sheet in the main window (or: loads in the window an existing parameters document).

Save: this command saves the parameters sheet shown on the screen to a disk file. If the parameters window has the default name "Untitled", UpenWin will open the *Save As* dialog box to let you rename the file and save it in a different directory or on a different drive.

Save As: this command lets you save the active parameters sheet to a file with a different name, in a different directory, or on a different drive.

Close: this command unloads the file in the active window and closes the window itself.

Print: this command displays the Printer Options dialog box which lets you print the contents of the window.

Print Preview: this command lets you see an on screen preview of how the parameters sheet will appear on printed page.

Print Setup: this command displays the system Printer Setup dialog box where you select which printer you want to use for printing with UpenWin. This command is disabled if no printer can be detected.

Exit: this command exits UpenWin, removes it from memory, and returns your Windows desktop.

Edit

Undo: this command restores the data in the current parameters sheet to the way it was before the most recent edit or cursor movement.

Cut: this command removes the selected data block from your parameters sheet and places the data in the *Clipboard*.

Copy: this command places the selected data in the *Clipboard* and leaves the selected data intact.

Paste: this command takes data from the *Clipboard* and puts it into the current parameters sheet at the cursor position.

Select All: this command selects the entire contents of the Edit window.

Find: lets you type the text you want to search for in the active Edit Window.

Find Next: repeats the last Find command.

Replace: this command displays the Replace Text dialog box, where you type in the text you want to search for and the text you want to replace it with.

View

Toolbar: check this menu item to turn on/off the toolbar (speed buttons).

Status Bar: check this item to turn on/off the status bar (or status line).

Run

Upen: by this command you can run a Upen computation session. A dialog box will be opened where you can select a data file to process.

2 Columns Filter: by this command you can run the program filter to convert a generic 2 columns data file format to the input format for Upen. A dialog box will be opened where you can select a data file to convert.

Upen Parameters

Most Adjusted: this command opens a dialog box where you can adjust the Most Adjusted Parameters.

Less Adjusted: this command opens a dialog box where you can adjust the Less Adjusted Parameters.

Seldom Adjusted: this command opens a dialog box where you can adjust the Seldom Adjusted Parameters.

Restore Defaults: this command restores all the Upen Parameters to the defaul

Help

Contents: this command displays the UpenWin online Help contents.

About Upen: this command displays the About UpenWin window which shows copyright and
version information.

Uninstall UpenWin

You can perform the uninstallation procedure in one of the two following ways (before performing the uninstallation be sure to close the program):

Uninstalling using *Uninstall UpenWin* Start Menu item
1. Click: Start > Programs > UpenWin > Uninstall UpenWin;
2. Follow the prompts.

Uninstalling using *Control Panel* (dependent on Windows version and configuration)
1. Click:Start > Programs > Settings > Control Panel > Add/Remove Programs;
2. Click UpenWin;
3. Follow the prompts.

Post-Uninstall
> The uninstallation removes all the installed files and settings, but leaves its directory, and the files put in it after installation, in place (on the machine), you will have to manually delete these files and the directory when uninstallation process is finished.

Most Frequently Adjusted Parameters

The following is a list of these parameters and their functions. These can be adjusted in the parameter file (click "par" with the folder symbol), and some can be adjusted also from the keyboard during computation (See "Keyboard Input"). They can also be adjusted under **UPEN Parameters – Most Adjusted**.

FileChr$	The output files (.dat and .tst) use the file name stem, plus one added character that permits computation for several choices of parameters, including some automatic choices based on some of the input control parameters, without overwriting previously-computed outputs. (*not* adjustable from the keyboard during computation).
	Permitted input values:
	  " " blank character for default output file symbol;
	  "J" to "Z" for non-default output file symbol, some symbols OK.

NNN$	No Non-Negative constraint. The data for many, but not all, relaxation time distributions have physical reasons for the distribution to be non-negative. The NN constraint can be lifted for exceptional cases or to investigate aspects of data quality also adjustable from the keyboard during computation, see Keyboard Input.
	Permitted input values:
	  " " or "y" for starting NoNN constraint;
	  "p" permanent NoNN constraint and disable undershoot feature (USHT$);
	  "n" does not permit NoNN constraint (permits NN).

MN$	Controls the choice of whether Sinf, the value of the fitted signal at infinite time, is included as a regression variable (*not* adjustable from the keyboard during computation).
	Permitted input values:
	  " " for auto, (from certain preprocessing only) the program decides automatically, , MN=1 for T_1 data and MN=0 for T_2 data;
	  "n" for no;
	  "y" for yes;
	  "i" a value of Sinf is request of the user.

AvNa$	("Av" for "average"; "Na" for "Number averaged") It is possible to use the first Na (normally =16) midpoints of successive signal pairs instead of the signals themselves. This is to mitigate the effects of instrument adjustment problems that lead to the alternation of early data points about any smooth fit. It can be set to be on or off or to be called automatically when the problem is detected (*not* adjustable from the keyboard during computation).
	Permitted input values:
	  "n" for no;
	  "y" for yes;
	  " " automatic (when RmR12 is high (>.05) uses the first Na midpoints).

beta000	This controls the starting value of a compliance parameter beta00, where larger values of beta00 (also adjustable from the keyboard during computation, see "Keyboard Input") allow more detail (not necessarily valid) in the computed fit. **Default value:** "1" (should usually not be more than 2).

AbsVal0$	This allows a number of options when absolute-value ("Modulus") data are being processed (*not* adjustable from the keyboard during computation). There is a wide range of data conditions and data problems.
	Permitted input values:
	  " " for no (default);
	  "y" for yes;
	  "i" a value for the absolute-value asymptote (asym) is requested of the user;
	  "a" for auto, if *Sinf* is positive and comparable to RumV treats data as absolute-value data;
	  "b" as "a" but the final computation will be done disenabling *Sinf* regression;
	  "c" as "b" but *asym* is evaluated from the single-channel noise;
	  "d" as "y" but *asym* is evaluated from the single-channel noise;
	  "e" as "d" but asks the user for an estimated baseline input (avblc).

MI	The number of logarithmically-spaced output relaxation times for which the distribution of relaxation times is computed (*not* adjustable from the keyboard during computation). MI is often about 100, but in some cases good data with sharp features can be improved by more

	points (and more computation time). **Default value:** "100".
ND	Number deleted of the shortest-time data points (*not* adjustable from the keyboard during computation). ND plus any previously-deleted points must be less than 1/D for windowed CPMG data. **Default value:** "0".
Mint	MINimum t, where t is data time (as opposed to relaxation time, T). Data points with t<Mint are discarded in the computation (*not* adjustable from the keyboard during computation). Must be well under TE/D for windowed CPMG data. **Default value:** "0".
Maxt	MAXimum t. Data points with t>Maxt are discarded in the computation (*not* adjustable from the keyboard during computation). **Default value:** "0".

Emx	Error-MaXimum. Some data sets may have points with "spike" noise, that is, a few points differing from an intermediate fit by more than the level of Gaussian random noise. These points can be automatically downweighted (*not* adjustable from the keyboard during computation).
	    "0" disables
	    "<2.5" disables except when AbsValue routines are used, in which case Emx=4 is used
	    "$\geq$ 2.5" points with Computed_signal_estimated/RumV >Emx are downweighted

Less Frequently Adjusted Parameters

Windowed\$	If data point spacing 1-2 is the same (now set as within 1%) as 2-3, UPEN assumes the data are T_2 data that are *windowed*, and it computes weighting factors according to data point times. "**n**" cancels the weighting and should be used for T_1 data with the first point spacings nearly equal or for T_2 data that have been "pruned" instead of windowed to have a manageable number of points for computation (or which have only a manageable number of points in the first place). "y" causes the data to be treated as windowed even if the first two intervals differ by more than the above 1%. This sometimes happens from severe truncation of digital data times. Also, for unknown reasons, there have been seen some low S/N data with lists of CPMG data times having intervals differing by as much as 35% and, in addition, having some double or zero steps. This can lead to the computation of totally wild weighting factors B(i), even giving negative ones that stop the program. A new feature is that setting Windowed\$ = "y" not only indicates windowing and weighting but also makes a stable approximate computation of the weighting factors for the windowed portion (usually after 2/D points), B(i) $\approx$ D*T(i)/TEE, where D is the relative window width (usually 0.05) and TEE is an average echo spacing.
	Permitted input values:
	        "y" windowed;
	        "n" unwindowed;
	        " " auto.

Tminn	Shortest output relaxation time if Tminn > 0; otherwise, shortest relaxation time is t (1)/LoXtrap, where **LoXtrap** is now 4. With Tminn=0, relaxation time components are allowed up to a factor LoXtrap below the first data point, but they are discouraged by the amplitude penalty unless the SNR is very high.
Tmaxx	Longest output relaxation time if Tmaxx > 0; otherwise, longest relaxation time is t(N)

	*HiXtrap, where **HiXtrap** is now 4. With Tminn=0, relaxation time components are allowed up to a factor HiXtrap above the last (N-th) data point (actually, the (N-SZ)-th data point if SZ≠0), but they are discouraged by the amplitude penalty unless the effective SNR is high.
TimeFact	Multiplies data time by this factor. Convert μs to ms, s to ms, etc. Times are usually given in ms in UPEN, and the screen display is labeled appropriately for ms.
SigFact	Multiply signal by this factor for convenience in tables or plots.
BulkFl\$	There is now an option to output also a distribution of relaxation times for fluids in porous media **corrected for bulk fluid relaxation**, having in mind that the relaxation rates are sums of the bulk fluid rate and a surface contribution proportional to *local* ratio of surface area to pore volume. If it can be assumed that both the surface rate and the bulk rate are significant, it may be useful to show a distribution of rates or times corrected for the bulk rate in order to reflect more directly the surface phenomena of interest. There are two steps required. One is to limit the range of output computed relaxation times to some time less than the bulk time. Then the usual correction for bulk rate, $1/T_{corr} = R_{corr} = R_{meas} - R_{bulk} = 1/T_{meas} - 1/T_{bulk}$, is applied to the output distribution of relaxation times. The distribution amplitude *g* is multiplied by a factor to preserve area in the distribution, $g' = g(1 - T_{meas}/T_{bulk})$. When bulk fluid correction is invoked by **BulkFl\$ = "y"**, two additional columns are added at the *beginning* of the output .dat spreadsheet. The uncorrected distribution is shown also, but it should be remembered that the range of computed output relaxation times may have been restricted by invoking BulkFl\$. With **BulkFl\$ = "y"**, you are asked for the bulk-fluid relaxation time (Tb) and an "extrapolation" factor (Tbx). Then, the longest relaxation time allowed in the inversion is Tmaxx=Tb/(1+1/Tbx), that is, extending the bulk-corrected time to Tbx × Tb. The corrected curves are usually not satisfactory if the uncorrected curves extend to Tb or beyond. **Permitted input values:** 　　　"y" for Bulk fluid correction; 　　　"n" for no Bulk fluid correction; 　　　"" as "n".
USHT\$	UnderSHooT clipping: With a finite spacing of computed points UPEN cannot prevent the overshoot and undershoot that comes from abrupt changes, such as at sharp peaks. If a minimum in a distribution (between two peaks or a peak and a tail) is narrower than allowed by resolution criteria in UPEN-I, **USH** can be chosen to force monotonic descent from a peak for the distance **UshRch** (USH reach, usually 0.3 Nepers). By adjusting UshRch one can implement most of the features of the former MONOTONIC cycle in UPEN. **pltmt** limits number of iterations. In Windows UPEN there is sufficient memory to permit computation of more output relaxation times than the usual MI=100, giving more closely-spaced points, with less tendency for undershoot and overshoot. USH can be implemented or removed from the keyboard during computation. **Permitted input values:** 　　　"y" enabled; 　　　"n" disabled; 　　　" " as "n".
Valley	A utility, **Peak_Tgm**, detects "resolved" peaks (when NN, the Non-Negative constraint, is used) and gives their geometric-mean relaxation times and signal fractions (integrated signal divided by the extrapolated XSig) as **Resolved Peaks**. **VALLEY** is the maximum allowable height of the valley floor above zero, in units of total signal (XSig) divided by the number of computed channels (MI). VALLEY should usually be well under 1.0. Default is, at the moment, 0.3. It should not be set to zero, since NN does not *precisely* zero g(k). VALLEY = 0.01 would be effectively zero, and 0.1 is close.
ValleyMx	Maximum relaxation time to use in Resolved Peaks computation.
Comment\$	"y" gives a prompt for insertion of a comment or information to go into the .TST file.
Mute\$	"y" blocks a five-note musical sequence when computation is finished. With fast computers this sound is usually not useful unless a larger than normal number of output points is being computed.

Seldom Adjusted Parameters

(Don't monkey with them)

SZ	SZ = 1 prompts you to put in a virtual data point at zero time. It has been used to impose a virtual zero-eth echo for sets of CPMG data with different echo spacings. It might be used for a virtual point after inversion by a 180° pulse (if you have valid reason to know how efficient the inversion is). **Default value:** 0.
MargRes$	A single iteration at $\beta = 16$ to prevent hysteresis (different resolution of marginally-resolved peaks for increasing and decreasing compliance β). Setting MargRes$ = "n" saves the time for this iteration and for two or three following ones to recover from the iteration at higher compliance. However, it may lead to the non-resolution of peaks that should be marginally resolved. **Default value:** "y".
NoOvProt$	not used (it is maintained for compability reasons).
Outst$	"y" gives a printable output parameter and results file (.TST file).
continue$	not used (it is maintained for compability reasons).
SinfSbtr$	"n" to not subtract Sinf (S_∞) from Sig in ".dat" file for MN = 1 (regression on Sinf).
WghtClip$	limits the weighting factors for windowed T_2 data to that for the top third percentile for the distribution. (to avoid giving excessive weight to noise and baseline).
FdbkLim$	Uses the input factor **FbLimFac** for automatic limitation of feedback to the smoothing parameter in cases where the feedback would otherwise produce a line narrower than allowed by Eq. [14] of UPEN-I.
FbLimFac	See **FdbkLim$.**
FxdHwLim	Fixed Halfwidth Limit. Limits the sharpness of lines in a computed distribution to a halfwidth of FxdHwLim Nepers (Overrides FdbkLin$).
SnrEfMax	Maximum effective SNR used in computing weightings of points. This can limit sharpest detail without affecting smoothing of broader features.
FxdReg$	Bypasses variable smoothing coefficients, giving non-UPEN computation with prompt for

	fixed curvature smoothing parameter, usually adjusted by trial and error.
Betaa	Amplitude penalty compliance outside datarange (not normally changed).
Betap	Compliance for slope feedback (not normally changed).
Betac	Compliance for curvature feedback (not normally changed).
Na	If AvNa is called (automatically or by AvNa$ = "y"), average the first **Na** (Number averaged, normally 16) input data pairs, i.e., use midpoints. See AvNa$ under Most Frequently Adjusted Parameters.
LoXtrap	If Tminn=0, then the shortest output relaxation time is $t(1)$/LoXtrap (normally = 4), where $t(1)$ is the first data point time.
HiXtrap	If Tmaxx=0, then the longest output relaxation time is $t(N)\times$HiXtrap (normally = 4), where $t(N)$ is the last data point time.
ClpDat$	"y" sets negative values to zero in the .Dat files for spreadsheet and plotting if NN is used. The NN (non-negative) constraint does not constrain the output distribution amplitude to *exactly* zero, but only to a very small value. This uselessly extends the scale in plotting programs to negative values. See UPEN-I.
TlongPct	Percent of XSig (extrapolated signal) in cumulative signal at longer time to define TLong. (Negative intervals count negatively.)
OutDat$	"y" gives an output text file (.DAT) for spreadsheets.
Scale$	Continue to auto-scale peak to top of screen on screen display during iterations. The only reason not to set Scale$ = "y" is if the user needs to compare amplitudes quantitatively over a number of iterations without renormalization.
Trans1	Numbers of iterations (normally 7) for Transitions after first trial periods. For AvNa, AbsValue, etc.
Trans2	Numbers of iterations (normally 5) for Transitions after second trial periods, for beginning NN (Non-Negative).
REACH	The reach in Np of ln-relaxation-time for determining coefficients in program. The default value 0.01 is coded to give one k-step, that is, nearest neighbors, regardless of the computed output-point spacing. It is probably not useful to change this except for insight into the process.
PNLT0	In use of USH (undershoot-clipping utility) the penalty for an MT (MonoTonic, now implemented in USH) violation, that is, for slope in the wrong direction for an interval subject to MT. PNLT0 should be large enough that a long sequence of MT points does not drift, especially to negative values. If it is too large, the sign on the computed slope cannot be reliably computed in order to know if it is still necessary after some iterations.
PNL0	As above, but for NN.
Converge$	"n" blocks the CONVERGE utility that hastens convergence after many iterations. Controllable (on or off) from keyboard also.
EXITNUM	The number of consecutive iterations that must have a maximum absolute relative change in error of fit below a percentage, **EXITDIF**.
EXITDIF	See **EXITNUM**.
WORSTM	The parameter **WORST** must be less than WORSTM to exit. WORST is the largest change in g_k relative to its last previous value or noise.
WORSTN	is the number of consecutive times that WORST must be less than WORSTM for exit from

	iterative cycle.
PMINP	Minimum inflection-point-pair slope in (SNR)/Neper required for action in the subroutine UNDSHOOT. Not critical.

T_2 Filter (Preprocessing) Parameters for 2 Columns CPMG Data File Format

T2$ is used as the first character of the output file extension.

D   the T_2 Filter averages the data points in windows of width D relative to the central time, starting with point number approximately $2/D$, after which the central times increase by the factor $(1+D)$. The value of D can be chosen according to the minimum relative linewidth available for the given SNR (signal-to-noise ratio) and number of points. A value $D=0.05$ is the default value and is adequate for most data sets, but a smaller value can be used for very high SNR and many points (but beware of over-interpreting very high S/N data, which must be equally free of systematic errors for valid interpretation). In fact, $D=0.1$ is adequate for many purposes and gives fewer points to process. So long as D is well under the minimum relative half-width of the line (in either the distribution of relaxation times or that determined by the random noise, whichever is greater), and so long as the significant signal errors are either slowly varying in time (as for many kinds of systematic data errors) or limited to statistically-stationary Gaussian random noise, no significant information is lost by the windowing.

T_1 Filter (Preprocessing) Parameters for 2 Columns IR Data File Format

C\$ is used as the first character of the output file extension.

Input Data Files

The input data files for UPEN computation are text files, formed by one line of comment (transmitted to UPEN for sample description or other information, max 72 characters) followed by 2 columns of data corresponding, respectively, to the time (preferably in ms) and to the signal amplitude. The data times should be monotonically increasing. The two columns can be separated by one or more characters not in "0123456789.+-eE". In each line, any character before ":" or after "!" is ignored. These files are read by "**2 Col**" **Filters** and binary files of the form used as UPEN input are produced.

Example:

My comment line…
```
   1.00  -717.03
   1.13  -639.00
   1.29  -679.80
   1.46  -728.36
   1.66  -709.90
   1.89  -719.67
   2.15  -645.20
   2.45  -629.69
   2.78  -638.22
   3.16  -614.17
   3.60  -587.02
   4.09  -549.32
   4.65  -474.55
   5.28  -512.87
```
…
…

Output and Display

Output Files

Two output files are produced at the end of an UPEN run. The output file name stem is that of the input data file plus an additional character, which is chosen automatically on the basis of some parameters unless **Filechar$** (just one character, which can be a letter or certain symbols such as # or _) is not blank (null string), in which case the added character is **FileChar$**. For the automatically-chosen characters, the value is "A" if MN=1 and AvNa$ blank; "B" if MN=0 and AvNa$ blank; "C" if MN=1 and AvNa$ is not blank; "D" if MN=0 and AvNa$ not blank. Then, if a list of other parameters does not have the default values, each of the above letters is advanced by four; that is, "A" becomes "E", etc. The output file name extension is .dat for several forms of the computed distribution and for the input decay data (with Sinf, the value at infinite time, subtracted unless SinfSbtr$="n"), and the extension is .tst (testo: text, but avoiding the standard "txt") for a text file with a list of non-default input parameters and the list of computed quantities listed and described under "Display".

.tst Files

A text file with a list of non-default input parameters and the list of computed quantities listed and described under "Display".

.dat Files

These are text files for spreadsheet or plotting programs and consist of eleven columns, with each pair of successive columns separated by one comma and one or more spaces. The columns are **T** (relaxation time, with times equally spaced on a logarithmic scale), **Sig_Np** (amount of input signal per Neper, or factor of *e*, of relaxation time), **Rate#** (ordinal number of computed distribution value, starting at the lowest rate, or longest relaxation time), **Pct_Np** (percent of total extrapolated signal per Neper of relaxation time), **Cum_Pct** (percent of the total extrapolated signal having a longer relaxation time), **SigT** (signal, or data point, time: does not include points excluded by non-default values ND, Mint, Maxt), **E:SNR***xxxx* (individual data point error of fit relative to the noise; *xxxx* is S/N), **Sig** (input signal, with Sinf, the computed or input value of the signal at infinite time subtracted unless SinfSbtr$="n"), **SigCalc** (the fitted signal, corresponding to the computed distribution of relaxation times), **Range** (two numbers: the shortest and longest data times), **Zero** (two zeros: the last ttwo columns, two numbers each, are for easily placing marks of plotted distributions of relaxation times to show the range covered by the data).

Display

SCREEN DISPLAY AND DIAGNOSTICS
(in order of appearance, if present)

The current curve is plotted in black, the curve from the last previous iteration is plotted in red, and any part of the baseline not covered by one of these two curves in shown in green. This makes it easier to see small differences between the curves and small distances from baseline.

At each iteration the **RESULTS** part (second part) of the **.tst file** is shown on the screen above the plot. There are numerous items that appear only if they are relevant. We will go down the list of items that appear, or might appear if relevant.

The name of the **file being processed** and the complete **path and name of the output .dat file** are given. It is important to note the added letter before the dot (See above and also CC$ discussion). The **.tst file** has the same name except for extension.

Next appears "**_plt_**" with a number to the left and another to the right. The number to the right is the program variable **pltt** (names referring to "plot"), which is the iteration number. The number to

the left is the program variable **plt** which is the number of iterations since any reset. This number is reset at Trans1 (7 iterations at present) and Trans2 (five more iterations), the times of program transitions related to computations for the diagnostics. The number plt is reset also at keyboard entries that change program parameters that require an adequate number of iterations for readjustment, and it is now reset at the single high-compliance iteration to provide seed for marginal resolution (if MargRes\$ = "y").

Next is "**_Change_**", with a number on the left and one on the right. The number on the left is the percent change in error of fit for the last iteration. With present settings, the absolute value of this percentage must remain below 0.03 for six consecutive iterations. The number to the right is the largest fractional (not percent) change of any computed point relative to its amplitude-plus-noise since the last previous iteration. With present settings, the absolute value of this must remain below 0.03 for three consecutive iterations. By watching these numbers one can see when the program is likely to finish. If either of these is large in the final display or in the .TST file, it indicates that iteration has been interrupted or has not successfully converged.

Next is the SNR (signal-to-noise ratio), **S/Rv** = USig/RumV. "U" means unextrapolated and is the computed fit to the signal at the time of the first data point. RumV ("V" for Variation of local error of fit) is the noise value computed from errors of fit of second-nearest neighbors; it should be closer to the *random* noise, because slowly-varying errors of fit are suppressed. The SNR can be used in criteria given in UPEN-I for resolution of lines and line widths and also gives one measure of data quality.

If NN (Non-Negative constraint) is not being applied, **Neg%** is given; it is the integrated negative part of the computed distribution relative to the integrated total. If NN has been called by keystroke entry, then "**NN_called_by_key**" is printed. If both transition iterations have been passed (7+5 at present), then **XNeg%** is printed; it is the negative percent just before application of NN. If there are no sharp features to the computed distribution, Xneg% should be very small. Large values warrant careful review of all the diagnostics. See also under RumNewOld.

RmR is an important diagnostic**,** again with a number to the left and one to the right. The number to the left is **RmR** = R_{rv} = ln(Rum/RumV), which should normally be negative or at least not more than a few percent if positive, since the regression minimizes Rum, not RumV. To the right is **RmR12** = ln(RumV1/RumV2), where RumV1 is the noise computed from errors of fit of the first Na (Number Averaged, 16 at present) pairs of nearest neighbors, and RumV2 from second-nearest neighbors. This is a measure of the alternation of the early data points about a smooth fit to the data. This is sometimes found even when only even echoes are used for T2 data and sometimes even found in T_1 data. This is a common data problem, and it may not greatly affect the computed distribution if not excessive and if there are not large very short relaxation time components. A large RmR12 does, however, affect the statistics of the noise for the rest of the data range. The use of the first **Na** (= 16 at present) data midpoints instead of the points themselves does much to lessen this problem. The utility **AvNa** implements this. The quantity RumV (R_v), used in computing RmR, is noise computed from all pairs of second-nearest neighbors, where the contribution of a slowly-varying error of fit can often be minimized. This parameter works best when there are closely-spaced data points. Positive values of more than a few percent usually indicate some data problems. That is, the data are not ideal in the sense of corresponding to random noise plus the sum of positive exponential components within the range of times covered by the data.

The next item is "**_Extrap_**", with the number on the left giving the percent of the integrated signal extrapolated to times shorter than the first data time, and the number of the right giving the percent of the integrated signal extrapolated to times longer than the longest data time. UPEN gently suppresses extrapolation of a distribution beyond the range of the data. If SNR (Signal-to-Noise Ratio) and other factors are favorable, a distribution may be extended to shorter or longer times than covered by the data. This is indicated on the list of diagnostic information, for

example, by **3.2%_Extrap_12.7%**, with 3.2% of the total signal being at relaxation times shorter than the time of the first data point and 12.7% longer than the last.

Then **Beta00** is given, where beta00 is the compliance parameter, with higher values giving less smoothing of the computed distributions. In the program it begins as Beta000 (normally = 1) but may be increased from the keyboard (**H**) or decreased (**h**) in steps of factors of $2^{1/2}$ or set to any desired value by keystroke (**j**) entry. See under **Rum – Sinf**. Normally, values of beta00 much less than 1.0 give oversmoothing, and values much over 2.0 give undersmoothing, possibly giving more detail in the computed distribution than required by the data.

The number to the left of the next entry, "**_BusyMMod_**" , gives a measure of the sharpness and amount of detail; the number on the right is a measure of multimodality. The variable **Busy** is the square root of the sum of first-differences-squared divided by the sum of amplitudes-squared for the distribution (and divided by the spacing in Np), giving a measure of the sharpness of detail. **Mmod** is the sum of absolute-first-differences divided by twice the peak, giving a measure of multimodality. A value of 1.0 means unimodal. See UPEN-II.

For the **_DATA_** entry there are two numbers on the left if **TEE**>0, presumably indicating CPMG T_2 data, where TEE is the spacing (Time) of Echoes Employed (all echoes, even echoes, etc.). If the first three signal times are not evenly spaced, then TEE = 0. If TEE>0, then TEE is printed, and, after a colon (:), the first data time is given. Then, after **_DATA_**, the longest data time is given. If we see **.6:.9_DATA_1198**, the first number is TEE, the spacing of echoes used; the second is the time of the first data point as used in the computation (1.5 ´ TEE if AvNa has been invoked, possibly longer yet if some early points are omitted); the third is the time of the last data point. For T_1 data or T_2 data without windowing (windowed$ = "n"), the first number is omitted. It is worth paying attention to whether or not the features of interest are adequately covered by the data. On the plot on the screen the data range is shown by the black squares plotted just below the baseline.

AvNa appears if AvNa has been called, either automatically or by being specified by AvNa$= "y". The following number is the Rum12 value *before* AvNa was called.

Tlong is the relaxation time for which 3% of the signal is longer, the longest significant relaxation time. If (without NN) there is a negative peak at long times, this counts *negatively* towards the cumulative 3%.

Then, there is a list of interpolated times of the **Peaks**.

Next, if there are resolved peaks, is **Resolved_Peaks_Tgm** and the geometric-mean (g-m) times and signal fractions of the resolved peaks. See the control parameter **VALLEY**, which controls how low the floor of the valley between a pair of peaks must be for the peaks to qualify as resolved. The parameter ValleyMx is the longest relaxation time that is used in computing the g-m time of the longest peak.

If early points are equally spaced (**TEE**>0) but the data do *not* represent *windowed* CPMG data, **Windowed$** should be set to "**n**", and "**UnWindowed**" will appear on the screen. If AvNa is in effect, whether automatically or directly, then "**AvNa**" will be printed. If the UnderSHoot utility is in effect, "**USH**" will be printed. If relevant, several parameters related to utilities limiting excess detail, including TSNR, hwms, hwmm, HWLimNo, are given.

The entry **RumNewOld** has a number to the left and one to the right. The value of RmR12o before application of AvNa is printed with "AvNa" *if* AvNa has been implemented. The number to the left of RumNewOld is ln(Rum/Rumo); the number to the right is ln(RumV/RumVo).

The "o" means the "old" value, namely, just before implementation of NN, which is normally at the second transition (at present, iteration 12) and which may be called by the keyboard entry "n" (see KEYBOARD INPUT DURING COMPUTATION) at a later time if NN is not called for initially. The number on the left is the cost of NN in worsened error of fit, which should not be much over 0.01 unless sharp lines are involved in the computed distribution. If there are sharp lines, 12 iterations might not be enough to give a stabilized "old" value. Furthermore, there might be the case of marginal resolution of two lines, where NN is expensive. However, a large cost of NN is likely to mean data problems. See also under **Rum – Sinf** .

When sequences of data are processed (or reprocessed), it is often inconvenient to have the program warn that an output file already exists. If NoOvProt$ = "y", the Overwrite-Protect is disabled, and the warning "**NO_OVERWRITE_PROTECT**" is printed.

To the left of **_gmTra_** is the **g**eometric-**m**ean relaxation time of the computed distribution of relaxation times, and to the right is the **r**ate-**a**verage time.

If the CONVERGE utility has been called, **CONVERGE** is printed. See CONVERGE and KEYBOARD ENTRY.

If **AbsValue** has been implemented, "**AbsValue:asymp**=" appears. The first number is the asymptote chosen by the program. The second number is the number of data points useful in determining the asymptote. The third number is Sinfld, the "old" value of Sinf (signal at infinite time), the value before applying AbsValue. See the discussion of AbsValue in UPEN-II. If an <u>a</u>bsolute-<u>v</u>alue <u>b</u>ase<u>l</u>ine <u>c</u>orrection **avblc** is subtracted from the data before processing, it is then listed. See AbsValue$ under Parameters.

Three signal values are given around the printed "**_XSigU_**" . X means extrapolated to zero time; U means unextrapolated, that is, the fitted curve evaluated at the time of the first data point; the third is the difference between the first and last points, which is independent of the processing. If Sinf is input (for instance, = 0 for CPMG with phase cycling) Sinf is substituted for the last point.

Rum - Sinf The rms error of fit Rum is the number to the left of "**_Rum_**" ; RumV, the estimated noise level, is to the right. Then **Sinf** is given. If Sinf is computed for CPMG data (instead of being set to 0 or some other value), its value should be compared to the noise value, RumV. If it is comparable to RumV, the possibility of absolute-value data should be considered. An example is **.06864_Rum_.05797 Sinf=-.0395,** where the first number is Rum, the second is RumV, and Sinf follows separately. If one suspects a legitimate marginal resolution of lines, it can be instructive to plot Rum (not RumV) as a function of beta00. This can be done fairly efficiently by starting UPEN with the usual beta000 = 1 and, after an iteration, pressing "g" to prevent iteration from terminating. After getting a solution (negligible further change), record such parameters as beta00, Rum (number on left), RmR (number on left), and RumNewOld (number on left). Then press "H" to increase beta00 by a factor of $2^{1/2}$ (or "h" to decrease beta00 by a factor of $2^{1/2}$). An abrupt improvement (decrease) of Rum for a small increase in beta00, accompanied by resolution of features, may suggest marginal resolution of features.

The **kurtosis** of the errors of fit is given. Values over 1.0 indicate outliers, or deviations from a Gaussian distribution of errors of fit. A substantial deviation probably indicates systematic data errors. The second kurtosis value is based on error differences of second-nearest neighbors.

If the error relative to noise |E(k)|/RumV >EMX>2.5 (See under EMX), Then "Downweight#" is printed, followed by the point number and, in parentheses, the data time.

If the Undershoot Protection utility USH is used, a list of output points for which slope is

forced to nearly zero is shown on the screen after the utility has started to operate.

WARNING – BEWARE

WARNINGs are given in orange print on the screen if any of the diagnostic parameters suggest special attention to possible data problems. Somewhat arbitrary levels of several parameters are chosen as a basis for the warnings. For even larger values of the parameters a **BEWARE** list is given in red. These levels are subject to change, but at present the values shown in the following table are used:

Diagnostic	Warning	Beware
Xneg%	18	30
RmR	0.05	0.15
RmR12	0.12	0.3
Xtrap	10	25
RumNewOld	0.05	0.12
$|Sinf|$ / Rum	0.3	
beta00	<1 or >2	<0.2 or >4
kurtosis	1	2.5

In addition notices regarding specific conditions or events are given, for instance, AvNa and AbsValue.

Miscellaneous

Keyboard Input

KEYBOARD INPUT DURING COMPUTATION
(Case-Sensitive, one key input per iterative cycle)
(Last input of cycle is used)

Press **f**	(fermare: to stop) to exit the iterative loop at the end of the current iteration and output results, whether or not the computation is finished.
Press **q**	(q: Quit) exit without writing output files, which will have been erased. This is to avoid file clutter.
Press **g**	to continue iteration regardless of computed exit criteria. Pressing f or q later will cause exit.
Press **+ (-)**	to call (cancel) the CONVERGE utility. After many iterations the solution usually converges, but it may wander or jump between two solutions that are not significantly different. After many iterations the CONVERGE utility is invoked and retains the weaker smoothing of the current and previous iteration, giving rapid convergence.
Press **A**, **B**, **C**, **D**, **E**	to magnify screen display a power of 2; A,B,C,D,E give factors of 2, 4, 8, 16, 32 (currently not much used).
Press **a**, **b**, **c**, **d**, **e**	to reduce screen display a power of 2; a,b,c,d,e give factors of ½, 1/4, 1/8, 1/16, 1/32. (currently not much used).
Press **U** (**u**)	to implement (remove) USH, the UnderSHoot-clipping utility. This utility clips an "undershoot" minimum next to a sharp peak with a tail, avoiding the appearance of the tail as a separate peak. The length of the protected interval can be controlled by the parameter UshRch. However, for good data, the minimum can often be avoided (at the expense of longer computation time) by increasing the parameter MI, the number of output points computed.
Press **y** (**n**)	"y" implements NoNN (which cancels NN, the Non-Negative constraint); "n" gives NN. Resets the iteration counter, plt.
Press **H** (**h**)	to multiply (divide) beta00 by square-root of two. Resets the iteration counter, plt. Larger beta00 (compliance parameter, normally 1.0) may give increased detail, possibly excessive, in the computed distribution.
Press **j**	for input prompt for exact value of beta00. Resets the iteration counter, plt. Larger beta00 (compliance parameter, normally 1.0) may give increased detail, possibly excessive, in the computed distribution.
Press **p** or **P**	Pause. Press any key to continue. This gives time to decide on any parameter changes from the keyboard.

UpenWin Tutorial

On double-clicking the UpenWin icon there are the buttons for T_1 and T_2 data Filters (2 Col) and UPEN. In addition there is access to Parameter settings for the Filters and for Upen. Files for input to UPEN are output from a 2 Col filter. The Parameters for the Filters and for UPEN are listed and described in Help, and the 2 Col filter format is also described.

## T_1 Example #1 – File T1Test1.001 (T1Test1.zip)

Running the 2-Col T_1 filter

Open and process the example file T1Test1.001 to obtain T1Test1.u01. The only parameter to set is the choice of letter to go in the position of the "u".

Running UPEN

Remember that for a T_1 relaxation data file it is almost always necessary to include the fitted signal at infinite time (Sinf, S_∞) as a regression parameter (See parameter MN$).

The file ending in h.DAT is the computed T_1 distribution, given in several forms for plotting. The file ending in h.TST is a text file of computed quantities and of several input parameters, including most non-default parameters. In the displays shown below, the initial processing was with default parameters. The effects of some variations in parameters used will be noted.
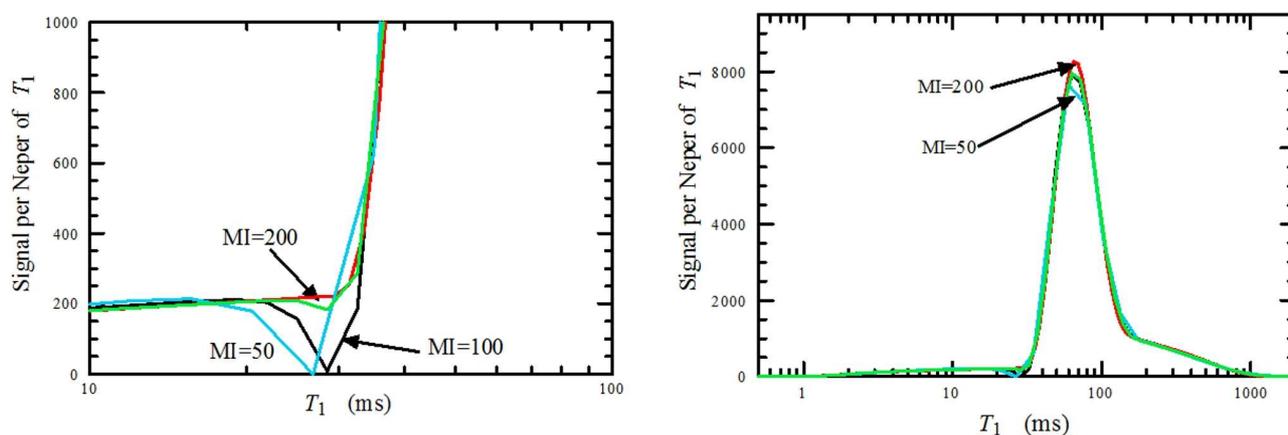
The distribution has a small tail extending to much shorter times and a substantial shoulder (or unresolved peak) at longer times. The figure at the left is a blow-up of the distribution at the right in order to show an artifact of filters in general, whether hardware or software, in which a sharp change in a distribution tends to give undershoot and overshoot. In our example, with the distribution computed for the usual MI=100 output relaxation times, there is a region of undershoot at the transition between the long low tail and the relatively sharp peak. With output points more closely spaced, by setting MI=200, the undershoot goes away. With MI=50 it is worse than for 100. The curve just below the arrow for MI=200 (without room for another arrow) is for MI=100 but using the Undershoot clipping utility (See parameter USHT$). Use of large MI greatly increases processing time, perhaps roughly as $(MI)^3$.

In addition to the .DAT files, from which the above figures were plotted, there is output a .TST text file with some information from the SDF header and information on some Parameters, including ones set to non-default values. Then there are computed values related to the data, including quantities that are hoped to have diagnostic value for identifying various data problems. These Display quantities are also identified in Help. The following is the TST file.

    T1TEST1.HDF Run:UPEN3E3_E14 07Aug2007 15:57 by T1sdf5b_e01.TRU 07Aug2007 SMPL= maiale6 EXP =   IR/S [DefaultSequence
    N=128 MI=100 NB=128 MN=1 beta000=1
        T1TEST1.HDF C:\TBF\Villiam\Test1\\T1TEST1H.dat 15_plt_27   -0.000%_Change_+0.007   S/Rv=279   XNeg%=1   -.065_RmR_+.038   0%
    _Extrap_0% beta00=1   1.94_BusyMMod_1.03 .1_DATA_3200 TLong=405 Peaks: 66.4 18.35 Resolved_Peaks_Tgm ;83.2,.946;7.86,.0536
    +.007_RumNewOld_+.000 73.9_gmTra_45.6 8281_XsigU_8263:8262 27.77_Rum_29.63 Sinf=-5.28 Kurtosis_-.43; -.76

The first line gives original file name and some processing and source file information. The first part of the second line is sample and experiment information from the SDF header. Then, N is the number of T_R values, that is, the number of T_1 data points. MI is the number of computed points on the T_1 distribution. NB is the number of original points if data windowing has been done, as for T_2 data; here it is the same as N. MN=1 means that the fitted signal Sinf at infinite time is a regression variable; MN=0 would mean that it is not. beta000=1 is the normal value of the starting compliance for regulation of inversion; see Parameters in Help. The third line gives the input data file name and the output .DAT file path and name. Then, there are numerous computed quantities, with the display showing only ones that are relevant. They are described more completely in Help under Output and Display.

To the right of plt is the number of iterations and to the left is the number of iterations since the iteration-exit criteria have been reset. Change is % change in error of fit in the last iteration (left) and biggest output change (right). S/Rv is the signal-to-noise ratio. XNeg% is the percentage of total signal in any negative peaks just before NN (non-negative constraint) is imposed.

RmR (R for "Rumore" or "Rauschen", Noise, but not starting with "N") is an important diagnostic quantity, again with a number to the left and one to the right. The number to the left is **RmR** = R_{rv} = ln(Rum/RumV). Rum is rms error of fit and RumV (V for Variation) is error of fit computed from error differences of nearest neighbors, reducing effects of slowly varying fitting errors. RmR should normally be negative or at least not more than a few percent if positive, since the regression minimizes Rum, not RumV. To the right is **RmR12** = ln(RumV1/RumV2), where RumV1 is the noise computed from errors of fit of the first Na (Number Averaged, normally 16) pairs of nearest neighbors, and RumV2 from second-nearest neighbors. This is a measure of the alternation of the early data points about a smooth fit to the data and is sometimes found even when only even echoes are used for T_2 data and sometimes even found in T_1 data. This is a common data problem, and it may not greatly affect the computed distribution if not excessive and if there are not large very short relaxation time components. A large RmR12 does, however, affect the statistics of the noise for the rest of the data range. The use of the first **Na** data midpoints instead of the points themselves does much to lessen this problem. The utility **AvNa** implements this. The quantity RumV (R_v, used in computing RmR, is noise computed from all pairs of second-nearest neighbors, where the contribution of a slowly-varying error of fit can often be minimized. This parameter works best when there are closely-spaced data points. Positive values of more than a few percent usually indicate some data problems. That is, the data are not ideal in the sense of corresponding to random noise plus the sum of positive exponential components within the range of times covered by the data.

The value of RmR (number on left) shown above is −0.048, a small negative value suggesting good data. The value on the right is +0.043, which is positive and indicates a mild alternation of the first few points about a smooth fit, is not high enough to automatically call AvNa (see AvNa$) or to lead to a WARNING message or the BEWARE message.

Extrap% gives the percent of total signal at times before the first data point or after the last.

beta00 (β) is the regulation compliance used in the final computation (as opposed to its initially-set value, beta000), and beta00 can be changed from the keyboard during computation (See Help, Keyboard Input). Restraint and careful attention to data quality and conditions are warranted when one considers increasing β much above the default value of 1.0 in order to show more detail in a distribution (or to decrease it much to get rid of unwanted detail). The increased detail acquired by increasing β is not valid unless there is a significant corresponding decrease in Rum (R_r in UPEN-II, significance criteria given in UPEN-I). Rum as a function of β (using MI=200) for the Liquid component of the signal from T1test1.SDF is easily found by pressing "g" during computation to continue iteration without exiting, then repeatedly pressing "j" to allow input of another β value (followed by Enter) and waiting for the Rum value to settle, as shown in the Table below.

beta00 (β)	0.125	0.25	0.5	1	2	4	8	16	32
Rum (R_r)	25.25	23.14	22.61	22.44	22.37	22.33	22.30	22.27	22.23

The minimum between the peak and the long tail on the left does not reappear (with MI=200) until β=16, and the shoulder on the right does not become a separate peak until β=32. The decrease in Rum obtained by increasing β above 1.0 is negligible. For some data sets the increase of β may sharply increase detail in the distribution without significantly decreasing Rum, in which case the data do not support the increased detail. However, there are cases of marginally resolved peaks where a small increase in β gives significantly more detail *and* significantly decreases Rum. Decreasing β below 0.5 does significantly increase Rum.

The number to the left of **_busymod_** is a measure of the amount of detail in the distribution, and the number to the right is 1.0 if the distribution is unimodal and higher if the distribution has more than one maximum.

Our example is for T_1 data, for which case the number to the left of **_DATA_** is T_R for the first data point and the number to the right is that for the last. However, it should be noted that for T_2 processing, for the **_DATA_** entry there are two numbers on the left if **TEE**>0, presumably indicating CPMG T_2 data, where TEE is the spacing (Time) of Echoes Employed (all echoes, even echoes, etc.). If the first three signal times are not evenly spaced, then TEE = 0. If TEE>0, then TEE is printed, and, after a colon (:), the first data time is given. Then, after **_DATA_**, the longest data time is given. If we see **.6:.9_DATA_1198**, the first number is TEE, the spacing of echoes used; the second is the time of the first data point as used in the computation (1.5 × TEE if AvNa has been invoked, possibly longer yet if some early points are omitted); the third is the time of the last data point. For T_1 data or T_2 data without windowing (windowed$ = "n"), the first number is omitted. It is worth paying attention to whether or not the features of interest are adequately covered by the data. On the plot on the screen the data range is shown by the black squares plotted just below the baseline.

TLong is the time for which 3% of the distribution is at longer relaxation time. **Peaks** shows a list of the interpolated relaxation times at the peaks of the distribution. The .TST file for the UPEN distribution (not shown) using MI=100 lists two peaks because of the baseline point due to undershoot. I addition there is the following display:

```
Resolved_Peaks_Tgm ;83.3,.946;8.41,.0544
```

Tgm means the geometric-mean relaxation time ($\exp<\ln T_1>$) for the peak. The above display means that the longer-time peak is at Tgm = 83.3 ms and has 94.6% of the signal and that the shorter-time "peak" is at 8.4 ms and has 5.4% of the signal. However, the shorter-time "peak" has been artificially "resolved" by undershoot. Also, it should be noted that the shoulder on the right of the main peak is included in its Tgm computation. (There is a means of excluding a feature at long times; see Parameter Valleymx.)

The entry **_RumNewOld_** has a number to the left and one to the right. The value of RmR12o before application of AvNa is printed with "AvNa" *if* AvNa has been implemented. The number to the left of RumNewOld is ln(Rum/Rumo); the number to the right is ln(RumV/RumVo). The "o" means the "old" value, namely, just before implementation of NN, which is normally at the second transition (at present, iteration 12) and which may be called by the keyboard entry "n" (see KEYBOARD INPUT DURING COMPUTATION) at a later time if NN is not called for initially. The number on the left is the cost of NN in worsened error of fit, which should not be much over 0.01 unless sharp lines are involved in the computed distribution. If there are sharp lines, 12 iterations might not be enough to give a stabilized "old" value. Furthermore, there might be the case of marginal resolution of two lines, where NN is expensive. However, a large cost of NN is likely to mean data problems. See also **Output** under **Rum – Sinf** .

The entry **_gmTra_** gives different average relaxation times for the whole distribution, Tgm is geometric-mean and Tra is rate-average (harmonic average, $1/<1/T_1>$).

Three signal values are given around the printed "**_XSigU_**". X means extrapolated to zero time; U means unextrapolated, that is, the fitted curve evaluated at the time of the first data point; the third is the difference between the first and last points, which is independent of the processing. If Sinf is input (for instance, = 0 for CPMG with phase cycling) Sinf is substituted for the last point.

Rum displays Rum and RumV as defined above under RmR. Rum is rms error of fit and RumV and RumV is estimated noise. **Sinf** (S_∞) is the fitted signal at infinite time, whether computed as a regression parameter (as for most T_1 data) or manually input or assumed to be zero (as in many T_2 data). The **kurtosis** of the errors of fit is given. Values over 1.0 indicate outliers, or deviations from a Gaussian distribution of errors of fit. A substantial deviation probably indicates systematic data errors. The second kurtosis value is based on error differences of second-nearest neighbors.

The file for this example is a good set of T_1 data. If RmR were over +0.05 or RmR12 over 0.12, there would be a WARNING message.

WARNINGs are given in orange print on the screen if any of the diagnostic parameters suggest special attention to possible data problems. Somewhat arbitrary levels of several parameters are chosen as a basis for the warnings. For even larger values of the parameters a **BEWARE** list is given in red. These levels are subject to change, but at present the following values are used:

Diagnostic	Warning	Beware
Xneg%	18	30
RmR	0.05	0.15
RmR12	0.12	0.3
Xtrap	10	25
RumNewOld	0.05	0.12
|Sinf| / Rum	0.3	—
beta00	<1 or >2	<0.2 or >4
kurtosis	1	2.5

In addition notices regarding specific conditions or events are given, for instance, AvNa and AbsValue.

T_2 Filter - Example file T2Test.zip (T2Test.zip)

The test file T2Test.zip (zipped) is a data file for a sequence of five CPMG data sets with increasing τ values, 10, 10, 20, 40, 100 µs (T2Test1.001, T2Test2.001, T2Test3.001, T2Test4.001, T2Test5.001).
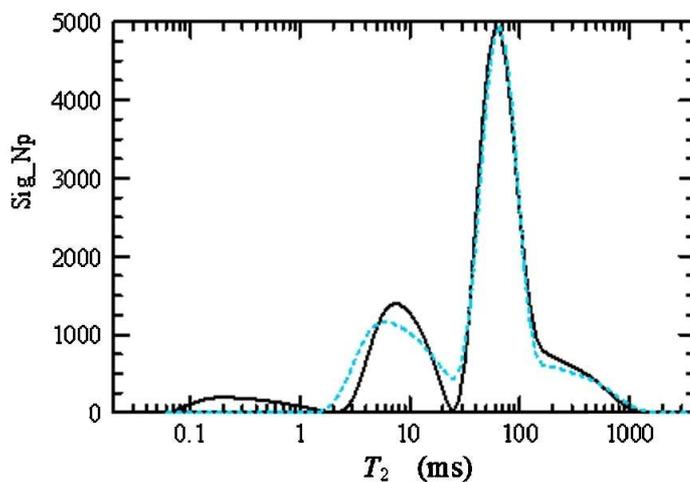
UPEN distributions from only the last two of these files are shown, since the shortest τ values give substantial contributions from a low-mobility component. The peak at about 0.2 ms on the solid black curve (τ=40) may possibly be of this origin. The dashed blue curve (τ=100) does not have a peak under 1 ms. It should be noted that the effective S/N is proportional to the square-root of the density of points, giving a ratio $(100/40)^{1/2}$ between the curves.