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EXAMPLES OF UNIFORM-PENALTY INVERSION OF MULTIEXPONENTIAL RELAXATION DATA

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When multiexponential relaxation data are inverted to give quasi-continuous distributions of relaxation times, the computed distribution is usually smoothed by means of an applied penalty function equal to a coefficient, *C*, times the integrated square of amplitude, slope, or curvature. When the distribution has a sharp peak and either a broad peak or long tail, smoothing with a fixed coefficient, *C*, widens the sharp peak and/or breaks up the broad peak or tail into two or more separate peaks. An iterative feedback procedure is used to generate a separate *C* value for each computed point in such a way as to give roughly equal contributions to the penalty function from each computed point. This permits adequate smoothing of broad features without oversmoothing sharp peaks. Examples are given for artificial data, for nuclear magnetic resonance in fluids in porous media, and for nuclear magnetic resonance in biological tissues. © 1998 Elsevier Science Inc.

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INTRODUCTION

In the inversion of multiexponential relaxation data it is normally necessary to apply some form of smoothing or "regularization" to the computed distributions of relaxation times to avoid solutions with excessive detail. A common way to limit detail is to minimize the sum of the squared errors of fit to which a penalty function has been added. The penalty function is often a smoothing coefficient, *C*, times the sum of the squares of the computed amplitudes, slopes, or curvatures. If the distribution has both a sharp peak and either a broad peak or a long tail, then most of the penalty is incurred by the sharp peak. Depending on *C*, the peak is broadened by local oversmoothing and/or the broad feature is broken into separate peaks, not demanded to be separate by the NMR data. We have for years dealt with this problem by "manually" imposing different *C* values[1] for a sharp peak and for a long tail or a broad peak.

We now use Uniform-Penalty (UP) inversion,[2] a less subjective approach to variable smoothing, in which the smoothing coefficient, C_k, for the k^{th} output point of the computed distribution of relaxation times is iteratively adjusted so that the penalty incurred at each point is roughly the same. The same iterative procedure is used to apply the usual non-negative (NN) constraint or monotonic (MT) constraint. Combinations of these constraints can be used to impose a monomodal or bimodal solution. MT can be applied to suppress "undershoot" in the vicinity of a sharp peak, which often leads to a narrower minimum than permitted by expressions for resolution.[2]

UP in its simplest implementation is neither efficient nor robust for relaxation data with high signal-to-noise ratio (s/n) and overlapping sharp and broad features. However, some reasonable limitations to changes after numerous iterations appear to stabilize the computation and lead to good results with artificial data. Furthermore, these circumstances are just those where other inversion methods give the problems of broadening a peak and/or breaking up a tail into several peaks.

EXAMPLES

Figures 1 and 2 show inversions of sets of synthetic relaxation data consisting of 127 points equally spaced in the logarithm of time from 0.2 ms to 10 s. The model is a sharp line at 310 ms and a rectangular tail contributing

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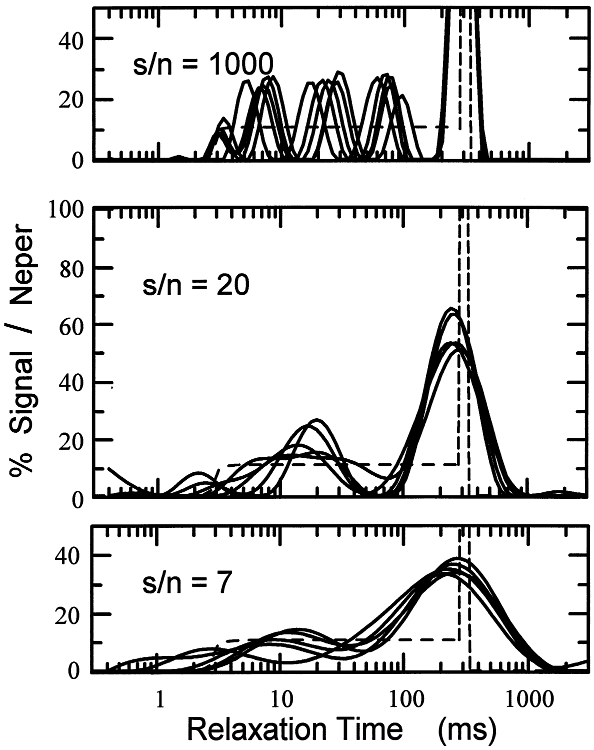

Fig. 1. Inversion of artificial relaxation data corresponding to the distribution shown by the dashed lines. At each s/n value, five datasets with different sets of random noise are inverted. The fixed smoothing parameters, *C*, give scatter appropriate for the noise. The s/n ratios apply separately to the sharp peak and the rectangular tail.

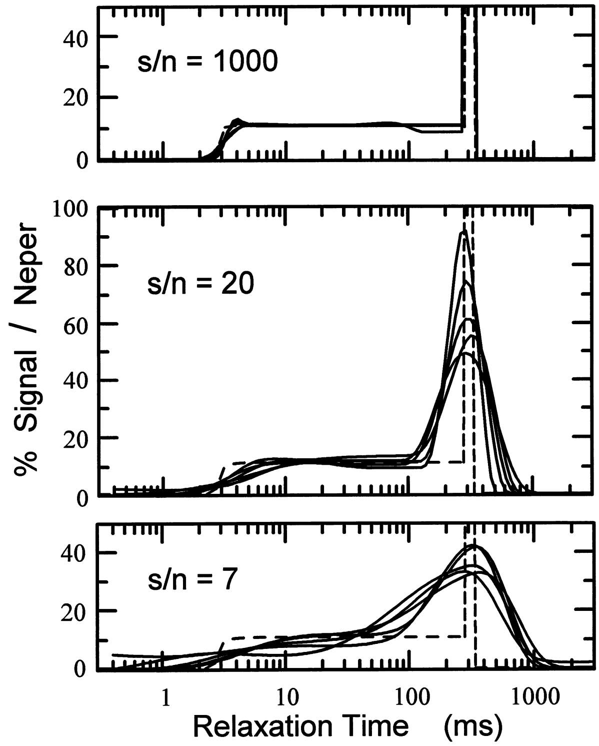

Fig. 2. Same as for Fig. 1, except that the UP inversion is used.

the same initial signal amplitude as the peak and extending from 3 to 310 ms. Different sets of random noise were added to each decay curve. The specified s/n values apply separately to the peak and the tail; that is, the overall s/n is twice the values noted. Five sets of data with the same model but with different sets of random noise were generated for each of three s/n values: 1000, 20, and 7. The fits have 110 points over the same time range as the data. The dashed line shows the model in Figs. 1 and 2.

Figure 1 shows fits, using inversion with fixed smoothing coefficients, *C*, chosen to give scatter appropriate to the added noise. At s/n = 1000, the *C* is too large for the peak, which is substantially broadened, leaving the peak width determined by the smoothing and therefore not varying with the five different sets of random noise. The same *C* is not enough to avoid breaking the tail into several apparent peaks. Furthermore, these peaks do not appear in the same places for different samples of the noise. At s/n = 20 apparent separate peaks are still produced. The main peak does not vary greatly with the five sets of added noise, because of the smoothing, but there is considerable variation in the apparent peaks representing the tail. At s/n = 7 there is only slight need for variable smoothing, but the distribution still tends to be split into two peaks when a fixed *C* is used.

Figure 2 shows fits to the same synthetic data, using UP inversion. For s/n = 1000 the five fits are very close to the model, the peak is only slightly broadened, and the tail is not broken into separate peaks. Even at this high s/n the fits are not identical. One fit is slightly lower next to the peak, and there is some variation at the beginning of the tail. In an additional series of 10 decay curves with different sets of noise (not shown) there was one that showed a peak with about twice the width of the rest, which is about the minimum that can be shown with the above spacing of the computed points.

The fits in Fig. 2 for s/n = 20 show more variation, with nearly a factor of 2 in peak widths. The peak widths are determined largely by noise and are therefore somewhat variable. However, the peak is still not broken away from the tail. For s/n = 7 the peak and tail are blended into one asymmetrical peak.

Figure 3 is for T_1 data for an oifield sandstone core cleaned and saturated with brine. The solid curve is with UP inversion, and the residual scatter is appropriate for the noise. The short dashed curve is for inversion, with a

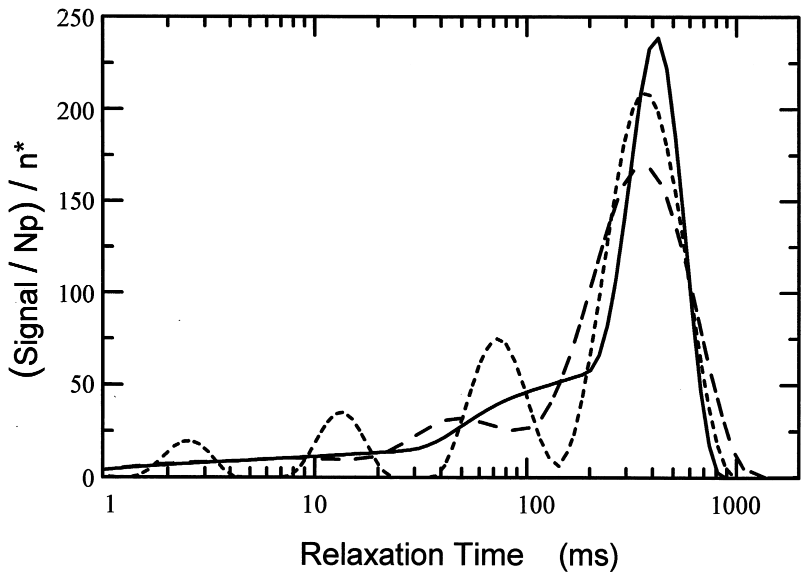

Fig. 3. Distributions of relaxation times for an oilfield sandstone core saturated with brine. The solid line is for UP inversion, and the short dashed line is for the fixed C giving the same scatter as that from UP. The long dashed line is with fixed C 100 times larger, giving a 7% increase in the scatter. The effective noise n^* is the rms added noise times the square root of the data point spacing in Np (Nepers).

fixed C chosen to give the same residual scatter as the UP fit. The peak is slightly broadened, and the tail is broken up into several apparent peaks. Increasing the fixed C by a factor of 100 gives a somewhat wider peak but an almost monotonic distribution. The scatter is increased by about 7%.

Figure 4 is for T_1 for a Berea sandstone cleaned and saturated with brine. The dashed curve is for UP inversion, and the five solid curves are for fixed C values at factors of 10, with the smallest C giving the narrowest and highest peaks. At first glance the smaller peaks might appear to be satellite peaks due to a low tail together with

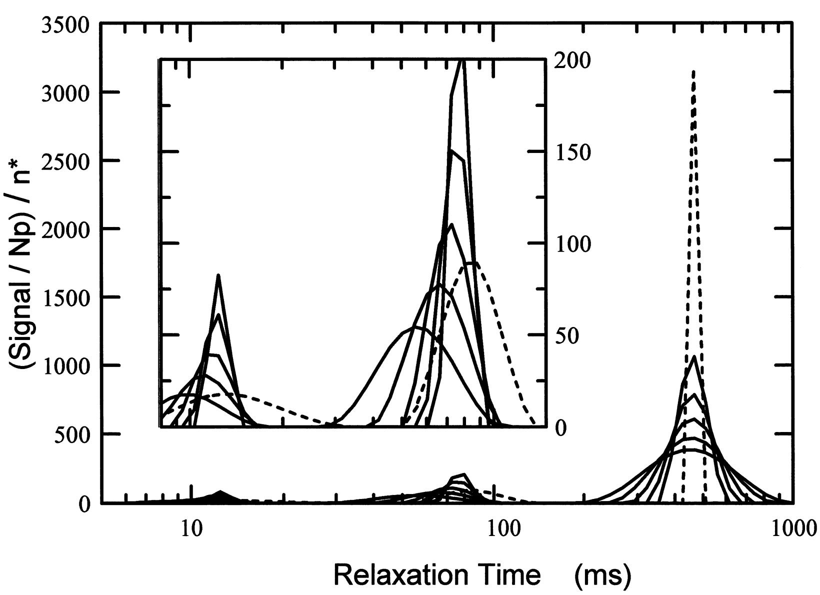

Fig. 4. Distributions of relaxation times for a Berea sandstone core saturated with brine. The dashed curve is from UP. The solid curves are for fixed C values at factors of 10. The least smoothing (highest curve for each of the three peaks) gives the same scatter as UP. The inset figure uses the same time scale as the main figure.

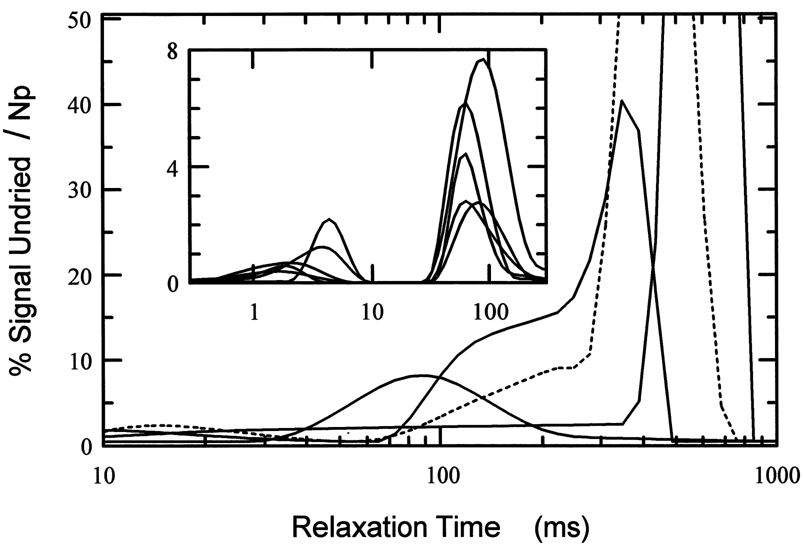

Fig. 5. T_1 distributions for bovine muscle tissue at various stages of drying. The solid off-scale curve is before drying, and the dashed curve is at 72% of the initial weight. The next lower curves are at 47% and 30%. The 30% curve is also shown as the highest in the inset, where drying is continued in steps down to 25% of the initial weight.

the undershoot occurring in the vicinity of a large peak. However, the peaks from fixed *C* inversion stay in nearly the same positions with different *C* values. Furthermore, UP processing with a monomodal constraint (not shown) increases the scatter by about 10%, which is enough[2] to make the continuous tail improbable. All of the main peaks from fixed *C* inversion are broader than those from UP. All of the smallest peaks from fixed *C* inversion are narrower than those from UP. All of the fixed *C* values, over a range of 10^4, are too large for the main peak and too small for the smallest peak. There is some overlap for the middle peak.

Figure 5 shows UP distributions of T_1 relaxation times for a sample of bovine muscle tissue. Measurements were made initially and after a series of periods of drying at 4°C in the presence of silica gel. The solid off-scale curve is before any drying and shows a long tail representing 7% of the signal. A fixed *C* inversion (fixed *C* curves not shown), giving slightly larger scatter, breaks the tail into four peaks, *permitted*, but not *required*, by the data. The dashed curve is at 72% of the initial weight. A fixed *C* inversion with slightly higher scatter isolates the short tail on the main peak as a separate peak, again *permitted* but not *required*. The larger on-scale curve in the main figure is for 47% of the initial weight. Here, fixed *C* inversion does not isolate the shoulder, but rather partly merges it with the main peak, because the main peak is widened. The remaining solid curve in the main figure is for 30% of the initial weight, and the peak just under 100 ms presumably includes signal from fat. The 30% curve is shown also as the highest curve in the inset figure, extending to shorter times and showing successively lower curves with further drying, with the lowest for 25% initial weight.

CONCLUSIONS

When a single distribution of relaxation times has both a sharp feature and a broad one, good representations of both can be obtained by inversion with a variable smoothing parameter. This can be determined by an iterative computation that tends to make the smoothing *penalty*, rather than the smoothing *coefficient*, roughly uniform along the distribution.

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