

● Short Communication

A METHOD FOR APPROXIMATING FRACTIONAL POWER AVERAGE RELAXATION TIMES WITHOUT INVERSION OF MULTIEXPONENTIAL RELAXATION DATA

G.C. BORGIA,* V. BORTOLOTTI,* R.J.S. BROWN,† AND P. FANTAZZINI‡

*Department of Chemical Mining and Environmental Engineering, University of Bologna, Viale Risorgimento 2, Bologna, Italy; †515 W. 11th St., Claremont, CA, USA; and ‡Department of Physics, University of Bologna, Via Irnerio 46, Bologna, Italy

A method is presented for approximating fractional power averages of relaxation times for data equispaced in log time, without the need to invert multiexponential relaxation data. This form of average permits giving emphasis to short or long times depending on the choice of the p value, thus giving the possibility of representing different specific properties of porous media. This method has been tested on a large number of nuclear magnetic resonance (NMR) relaxation measurements in porous samples. This new algorithm appears to be robust with respect to both measurement and computation, and its major advantage is that it does not depend on a particular inversion method. Moreover, it permits a very fast computation. © 1998 Elsevier Science Inc.

Keywords: Multiexponential nuclear magnetic resonance relaxation; Fractional power average time; Fast computation.

INTRODUCTION

In the nuclear magnetic resonance (NMR) relaxation studies of porous media it is often necessary to represent a wide distribution of relaxation times by means of a single parameter time. Some, but not all, methods involve the steps of resolving the data into a number of discrete exponential components or a quasi-continuous distribution of components to compute some forms of “average” time. The fractional p -power average $T^{(p)} \equiv \langle T^p \rangle^{1/p}$ is able to give various different emphases to long and short times, depending on the p value. In this paper we present a computation we call *Robusta* approximation (RA) that gives approximations $T_r^{(p)}$, or simply T_r , if p is specified separately, to $T^{(p)}$ without requiring the resolution of relaxation data into sums of exponential components. The method is a generalization of the RA computation for the geometric mean.¹

Here we present the computation based on a sequence of n data points S_i taken at times t_i at equal intervals in $\ln t$, where t is data time. We assume that t_n is long enough for substantially complete relaxation. An algo-

rithm is derived to show that $T_r^{(p)}$ is given by the implicit equation:

$$T_r \approx \left(\frac{1+p}{\Gamma(2+p)} [pge^{-t_0/T_r} + t_0^p f(t_0/T_r)] \right)^{1/p} \quad (1)$$

The symbols are defined below.

In a companion paper,² in which these computed times use 126 data points starting at 0.4 ms, it is shown that for $-1 < p < -0.3$ the approximation to $T^{(p)}$ is not very close, but T_r appears nevertheless to be a good form of “average” time for estimation of irreducible water saturation. The approximation is very close for p values closer to zero,² and therefore it is a good form for estimating permeability.^{2,3}

COMPUTATION

The integral $\int_0^\infty t^{p-1} S(t) dt$ gives the T^p -average relaxation time if t values are data times, T values are relaxation times, $p > 0$, and the relaxing signal $S(t)$ is normalized to $S(0) = 1$, $S(\infty) = 0$. That is, $\int_0^\infty t^{p-1} S(t) dt = \Gamma(p) \int_0^\infty T^p a(T) dT = \Gamma(p) \langle T^p \rangle$, where $a(T)$ is

Address correspondence to Dr. G.C. Borgia, Dept. ICMA, University of Bologna, Viale Risorgimento 2, 40136, Bologna, Italy

amplitude for a distribution of relaxation times. However, as $p \rightarrow 0$, it becomes impractical to take data at sufficiently short times to represent the integrals adequately. In the limiting case, as p approaches zero from either side, we have the RA to the geometric-mean time,¹ the neutral position between time and rate averages. For positive or negative fractional values of $p > -1$ we will generalize the RA.

The G Integral

In analogy with the RA to geometric mean time, consider the integral $G = \int_{t_0}^{\infty} t^{p-1} S(t) dt$, $S(t) = \sum c_i e^{-t/T_i}$, and $\sum c_i = 1$, where p is not zero or a negative integer. The T values are component relaxation times for multiexponential relaxation. The limit t_0 will be related to the shortest data time. We let $\sigma_i = t_0/T_i$. Using the dimensionless integration variable $\tau = t/T_i$, we have $G = \sum c_i T_i^p \int_{\sigma_i}^{\infty} \tau^{p-1} e^{-\tau} d\tau = \sum c_i T_i^p I(\sigma_i)$, where, for a fixed p , $I(\sigma) = \int_{\sigma}^{\infty} \tau^{p-1} e^{-\tau} d\tau$. For $p > 0$ and $\sigma = 0$, this is the Euler integral for the gamma function. For $-1 < p < 0$, one integration by parts gets us to the range of p where the integral from 0 to ∞ exists and gives the gamma function, but two integrations by parts get to the range easily found in tables. It is then useful to continue to integrate by parts to get a power series in σ :

$$I(\sigma) = -\frac{\sigma^p e^{-\sigma}}{p} - \frac{\sigma^{1+p} e^{-\sigma}}{p(1+p)} - \dots - \frac{\sigma^{m+p} e^{-\sigma}}{p(1+p)(2+p) \dots (m+p)} + \frac{1}{p(1+p)(2+p) \dots (m+p)} \int_{\sigma}^{\infty} \tau^{m+p} e^{-\tau} d\tau. \quad (2)$$

We let $\int_{\sigma}^{\infty} = \int_0^{\infty} - \int_0^{\sigma}$, with $\int_0^{\infty} = \Gamma(m+p+1)$ and $\int_0^{\sigma} = \sigma^p e^{-\sigma} O(\sigma^{m+1})$. Using the recursion relation $z\Gamma(z) = \Gamma(z+1)$ and neglecting the term in $O(\sigma^{m+1})$, we have $I(\sigma) \approx -(\sigma^p/p)f(\sigma) + \Gamma(2+p)/[p(1+p)]$, with

$$f(\sigma) = e^{-\sigma} \left(1 + \frac{\sigma}{1+p} + \frac{\sigma^2}{(1+p)(2+p)} + \dots + \frac{\sigma^m}{(1+p)(2+p) \dots (m+p)} \right) \quad (3)$$

$$G = -\frac{t_0^p}{p} \sum c_i f(\sigma_i) + \frac{\Gamma(2+p)}{p(1+p)} \sum c_i T_i^p, \quad (4)$$

because $\sigma_i = t_0/T_i$. We note that G does not exist for $p = 0$ or $p = -1$. We assume that sample relaxation times are covered sufficiently that $\sigma < 1$ in Eq. (3) and

note that more terms are needed in Eq. (3) as $p \rightarrow -1$. We do not know the σ_i values to use in $f(\sigma_i)$, but $f(\sigma_i)$ is fairly close to unity if the data extend to times well below the shortest significant component times, that is, $\sigma_i \ll 1$. If we substitute some fixed value T_{old} for T_i in σ_i , Eq. (4) becomes:

$$G \approx \frac{1}{p} \left(-t_0^p f(t_0/T_{old}) + \frac{\Gamma(2+p)}{1+p} \langle T^p \rangle \right) \quad (5)$$

The g Sum

For our data the signal is sampled with equal spacing in $\ln$ time. The step in time is by a factor of e^{2q} , where $q = [\ln(t_n/t_1)]/[2(n-1)]$, and the step in $\ln t$ is $2q$. We assume that $S_n = S(t_n) \approx S(\infty)$, and we normalize S so that $S_n = 0$ and $S_1 = 1$. We approximate the integral G by the sum g , with:

$$g = 2q \sum_{i=1}^{n-1} S_i t_i^p. \quad (6)$$

The time t_i for each sampled signal should be at the center of a corresponding interval from u_{i-1} to u_i in the integral G such that $\int_{u_{i-1}}^{t_i} t^{p-1} dt = \int_{t_i}^{u_i} t^{p-1} dt$. The ratio $u_i/u_{i-1} = e^{2q}$, giving $(u_{i-1}/t_i)^p = e^{-q}/\cosh(pq)$. The time t_0 for the beginning of the G integral is then:

$$\frac{t_0}{t_1} = \left(\frac{e^{-q}}{\cosh(pq)} \right)^{1/p} \approx \exp \left(-q - \frac{1}{2} pq^2 \right). \quad (7)$$

For G we normalized the signal to unity at $t = 0$ and zero at $t = \infty$. For the sum g the best we could do was to normalize to unity at $t = t_1$ and zero at $t = \infty$. We can partially compensate for this by multiplying g by $e^{-t_1/T_{old}}$, where, as in Eq. (5), T_{old} is an estimate. We now have:

$$G \approx \frac{1}{p} \left(-t_0^p f(t_0/T_{old}) + \frac{\Gamma(2+p)}{1+p} \langle T^p \rangle \right) \approx g \exp(-t_1/T_{old}). \quad (8)$$

Using Eq. (7) for t_0 , Eq. (3) for f , Eq. (6) for g , and either ∞ or some typical value for T_{old} :

$$T^{(p)} \equiv \langle T^p \rangle^{1/p} \approx T_{new} \equiv \left(\frac{1+p}{\Gamma(2+p)} [pg \exp(-t_1/T_{old}) + t_0^p f(t_0/T_{old})] \right)^{1/p}. \quad (9)$$

We use a simple approximation to the gamma function⁴ and iterate as necessary (ordinarily just once if $|p|$ is small) to get the RA $T_r = T_{new} = T_{old}$, which is Eq. (1). The dependence of the right side of Eq. (9) on T_{old} is weak, and a few iterations by using T_{new} from (9) in one iteration for T_{old} in the next give an easily computed result.

CONCLUSIONS

The relaxation time $T_r^{(p)}$ is well specified, it does not require inversion of relaxation data, and it is quickly computed despite involving one or a few iterative steps. It is a close approximation to $T^{(p)} = \langle T^p \rangle^{1/p}$ for small $|p|$, and even outside this range, it has given as good or better correlations² with S_{wi} and k than other forms of “average” relaxation times. An advantage of $T_r^{(p)}$ is that it does not depend on details of an inversion method.

Acknowledgments—This work was supported by University of Bologna (funds for selected research topics) and by Murst Grants.

REFERENCES

1. Borgia, G.C.; Bortolotti, V.; Brown, R.J.S.; Fantazzini, P. A robust method for calculating geometric mean times from multiexponential relaxation data, using only a few data points and only a few elementary operations. *Magn. Reson. Imaging* 14:895–897; 1996.
2. Borgia, G.C.; Brown, R.J.S.; Fantazzini, P. Estimates of permeability and irreducible water saturation by means of a new robust computation of fractional power average relaxation times. *Magn. Reson. Imaging* 16:613–615; 1998.
3. Borgia, G.C.; Brown, R.J.S.; Fantazzini, P. Different “average” nuclear magnetic resonance relaxation times for correlations with fluid-flow permeability and irreducible water saturation in water-saturated sandstones. *J. Appl. Phys.* 82: 4197–4204; 1997.
4. Press, W.H.; Flannery, B.P.; Teukolsky, S.A.; Vetterling, W.T. *Numerical Recipes*. Cambridge: Cambridge University Press; 1989.