

# Polynomial Solutions of Bloch NMR Flow Equations for Classical and Quantum Mechanical Analysis of Fluid Flow in Porous Media

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**Abstract:** In many NMR experiments it is noticed that liquids confined in porous materials exhibit properties that are different from those of the bulk fluid. Determining the relationship between macroscopic properties and the microscopic structure of porous materials and their components has been difficult. Despite decades of study, researchers' understanding is generally limited to empirical correlations based on laboratory measurements. Only recently have researchers been able to calculate a few of the macroscopic physical properties of rocks from first principles. In this contribution, we have presented polynomial solutions of the Bloch NMR flow equations for classical and quantum mechanical analysis of porous media applicable in oil and gas industry. The NMR polynomials are derived based on the condition that

$$\gamma^2 B_1^2(x) \ll \frac{1}{T_1 T_2}. \text{ We transform the transverse magnetization } M_y, \text{ into porous medium with a transformation con-}$$

stant  $a$ , which must be positive. The direction of the positive constant  $a$ , can only take on one of  $\vartheta = (2n+1)$  possible values. The lowest allowed value of  $a$ , with  $n = 0$  is not zero. This implies that, even in a very complicated porous medium, the lowest allowed value of  $a$  always has a  $T_2$  relaxation parameter. This is valid both in classical and quantum mechanical analysis of porous media. In addition to relating the porosity with depth, the mathematical procedure yield information on the dynamics of various parts of the porous media. The transverse relaxation rates  $R_{2n}$  are the eigenvalues of the porous medium with  $n$  as the quantum number. It determines the specific porous state which the fluid particles occupy within the pore. The state, and therefore  $T_2$  relaxation rate is quantized, determined by the quantum number  $n$  which is any integer greater than or equal to zero.

**Keywords:** Bloch NMR flow equations, Porous media, Quantum mechanics, Hermite polynomials, Porosity, Permeability and Poromechanics.

## INTRODUCTION

Generally, porous materials are (often called matrix) permeated by interconnected network of pores (voids) filled with a fluid. Examples include granular materials, foam, ceramics, animal lungs and sinuses, and oil-or water-bearing (reservoir) rocks. The understanding of the important properties of these materials, such as porosity, could reveal the nature of their geometry, permeability, the fluid they contain, the molecular interaction between the fluid particles and the surface of the pores. Nuclear magnetic resonance (NMR) has been very useful in the study of pore size distribution of these materials and also in molecular recognition. In fact, important properties of the porous media have been shown to be very much dependent on the  $T_1$  and  $T_2$  relaxation times [1-6]. That is, the NMR transverse magnetization carries information on the pores' properties. This has been demonstrated by many experiments on porous media [7-12], but analytical expressions showing the direct relationships between the pore features and the NMR parameters have been quite scarce in literature.

Since petroleum can only occupy the pore space, determining the formation porosity is of primary importance. A number of techniques including neutron and gamma – ray scattering, acoustic propagation, and magnetic resonance have been developed to measure porosity [7-16].

Although these instruments are limited to measuring proton relaxation of fluids in rock, they provide valuable information. One important relaxation mechanism is controlled by hyperfine interactions between protons in the pore fluid and unpaired electrons at the grain surface.

The resulting relaxation rate is proportional to the surface-to-volume ratio of the pore space. This ratio is controlled by the smallest dimension of the pore; therefore it is often said that the relaxation time,  $T_2$ , depends on the pore size.

Breakthroughs in measurement techniques and signal processing will be needed before hydrocarbon accumulations can be mapped in three dimensions with high spatial resolution [17]. Significant advances in the understanding of both multi-component flow in porous media and the physics of wettability are crucial for the development of technology to minimize bypassed oil [17-23].

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The main goal of this study is to establish a methodology of using mathematical techniques so that the accurate measurement of fluid flow in porous media can be carried out non-invasively and yet the technique would be easy and simple to implement. This is primarily applicable to locate hydrocarbon – bearing zones; to measure porosity, hydraulic permeability, and hydrocarbon viscosity; and to determine the fraction of water bound by capillary forces in small pores. The procedures can be applied to non invasive estimation of flow rates of any fluid (blood flow) in porous media that contains unpaired nuclear spins so that NMR signal of the fluid can be obtained.

We consider the fluid particle (on the atomic scale) which either initially or in some average sense is in steady rotation. We apply a mathematical algorithm to describe in detail the dynamical state of the flowing fluid particle starting from the Bloch NMR flow equations. We study the flow properties of the modified time independent Bloch NMR flow equations (shown in Equation (1)) which describe the dynamics of fluid flow under the influence of radiofrequency magnetic field as derived in the earlier studies [24-28].

$$\frac{d^2 M_y}{dx^2} + \frac{1}{V} \left( \frac{1}{T_1} + \frac{1}{T_2} \right) \frac{dM_y}{dx} + S(x)M_y = \frac{M_o \gamma B_1(x)}{V^2 T_1} \quad (1a)$$

where

$$S(x) = \frac{1}{V^2} \left( \gamma^2 B_1^2(x) + \frac{1}{T_1 T_2} \right) \quad (1b)$$

subject to the following conditions:

- i.  $M_o \neq M_z$  a situation which holds good in general and in particular when the radiofrequency (rF)  $B_1(x)$  field is strong say of the order of 1.0G or more.
- ii. Before entering signal detector coil, fluid particles has magnetization  
 $M_x = 0, M_y = 0$
- iii.  $B_1(x)$  is large;  $B_1(x) \gg 1G$  or more so that  $M_y$  of the fluid bolus changes appreciably from  $M_o$ .
- iv. for steady flow,  $\frac{\partial M_y}{\partial t} = 0$

In Equation (1),  $M_y$  is the transverse magnetization (the NMR signal),  $V$  is the fluid velocity,  $\gamma$  is the gyromagnetic ratio of the material,  $B_1(x)$  is the applied radiofrequency magnetic field,  $T_1$  and  $T_2$  are the spin-lattice and the spin-spin relaxation times respectively.

### The Transformation of NMR Transverse Magnetization into a Porous Medium

The NMR polynomials of Equation (1) would be derived based on the condition that

$$\gamma^2 B_1^2(x) \ll \frac{1}{T_1 T_2}$$

We apply the transformation [29, 30]  $M_y(x) = M_y(P)$  (transforming  $M_y$  into a porous medium with porosity  $P(x)$ ) such that:

$$\frac{dM_y}{dx} = \frac{dM_y}{dP} \frac{dP}{dx} \quad \text{and} \quad \frac{d^2 M_y}{dx^2} = \frac{d^2 M_y}{dP^2} \left( \frac{dP}{dx} \right)^2 + \frac{dM_y}{dP} \frac{d^2 P}{dx^2} \quad (2)$$

From Equations (1) and (2), we obtained

$$\frac{d^2 M_y}{dP^2} + A \frac{dM_y}{dP} + a^2 M_y = a^2 T_2 M_o \gamma B_1(x) \quad (3)$$

where

$$\frac{\frac{d^2 P}{dx^2} + \frac{1}{V} \left( \frac{1}{T_1} + \frac{1}{T_2} \right) \frac{dP}{dx}}{\left( \frac{dP}{dx} \right)^2} = A \quad (4a)$$

$$\frac{\frac{1}{V^2} \left( \frac{1}{T_1 T_2} \right)}{\left( \frac{dP}{dx} \right)^2} = a^2 \quad (4b)$$

provided that  $A$ , is a constant and  $a^2$  is any positive constant. For the purpose of obtaining fundamental (semi-classical and quantum mechanical) information about the variation of porosity with depth for fluid dynamic evaluation in porous media by means of the Schrödinger equation and the Hermite polynomials, it is very important in this analysis to choose  $A = 0$ . This allows us to discuss the dynamics of the NMR system in terms of harmonic oscillator, one of the most important model systems in quantum mechanics. The constant  $M_o$  in this case is the force constant. The larger the force constant, the larger the restoring force.

Based on condition (i) above, we consider the radiofrequency field in equation (2a) designed according to Equation (5).

$$\gamma B_1(x) = P^2 M_y(P) \ll \frac{1}{\sqrt{T_1 T_2}} \gg 1G \quad (5)$$

The physical application of Equation (5) can be demonstrated for blood flow ( $T_1 = 1\text{sec.}$  and  $0.001\text{sec.} < T_2 < 0.5\text{sec.}$ ) in restricted geometries. In the porous medium, Equation (3) can be written as

$$\frac{d^2 M_y}{dP^2} + a^2 (1 - T_2 M_o P^2) M_y = 0 \quad (6)$$

It is necessary to define another variable  $U(P)$  such that

$$U = (T_2 M_o)^{1/4} a^{1/2} P \quad (7)$$

Equation (6) becomes

$$\frac{d^2 M_y}{dU^2} + \left( \frac{a}{\sqrt{T_2 M_o}} - U^2 \right) M_y = 0 \quad (8)$$

We must find solutions for which  $M_y(x)$  and its first derivative are single valued, continuous, and finite, for all values of  $x$ . The first two conditions will automatically be satis-

fied by the solution of the requirement that  $M_y(U)$  remains finite as  $|U| \rightarrow \infty$ . For this purpose, it is useful, first to consider the form of  $M_y(U)$  for very large value of  $|U|$ . The quantity  $\frac{a}{\sqrt{T_2 M_o}}$  becomes negligible compared to  $U^2$  for

very large value of  $|U|$ . Equation (8) can then be written in the form

$$\frac{d^2 M_y}{dU^2} - U^2 M_y = 0 \tag{9}$$

The general solution of Equation (9) is

$$M_y(U) = D_1 e^{-\frac{U^2}{2}} + D_2 e^{\frac{U^2}{2}} \tag{10}$$

where  $D_1$  and  $D_2$  are arbitrary constants. Applying the condition that the eigen functions must remain finite as  $|U| \rightarrow \infty$ .

It is apparent from Equation (10) that the term  $D_2 e^{\frac{U^2}{2}} = 0$ . The form of the eigen functions for very large value  $|U|$  must be

$$M_y(U) = D_1 e^{-\frac{U^2}{2}} \tag{11}$$

Equation (11) suggests that the solution of Equation (8) should be in the form

$$M_y(U) = D_1 e^{-\frac{U^2}{2}} F(U) \tag{12}$$

For the solutions in Equation (12) to be valid for all  $U$ ,  $F(U)$  must be functions which are slowly varying compared to  $e^{-\frac{U^2}{2}}$  as  $|U| \rightarrow \infty$ . The differential equation that completely determines the functions  $F(U)$  was found to be

$$\frac{d^2 F}{dU^2} - 2U \frac{dF}{dU} + \left(\frac{a}{\sqrt{T_2 M_o}} - 1\right)F = 0 \tag{13}$$

By applying a power series of the form

$$F = \sum_{v=0}^{\infty} c_v U^v \tag{14}$$

We obtain a recursion relation

$$c_{v+2} = -\frac{\left(\frac{a}{\sqrt{T_2 M_o}} - 1 - 2v\right)c_v}{(v+2)(v+1)} \tag{15}$$

An acceptable solution of Equation (14) requires that  $F(U)$  is finite when the recursion relation terminates. Equation (15) terminates for a specific choice of  $\frac{a}{\sqrt{T_2 M_o}}$  and

$v = n$  such that

$$\frac{a}{\sqrt{T_2 M_o}} = 2n + 1 \tag{16}$$

where  $n = 0, 1, 2, 3, 4, 5, \dots$

and

$$c_{n+2} = -\frac{\left(\frac{a}{\sqrt{T_2 M_o}} - 1 - 2n\right)a_n}{(n+2)(n+1)} = -\frac{(2n+1-1-2n)a_n}{(n+2)(n+1)} = 0 \tag{17}$$

The coefficients  $c_{n+4}, c_{n+6}, c_{n+8}, \dots$ , will also be equal to zero since they are proportional to  $c_{n+2}$ . The resulting solutions  $F_n(U)$ , are polynomials of order  $U^n$ , called the Hermite polynomials [29, 31]. Each  $F_n(U)$  can be evaluated by finding the coefficients from the recursion relation with the value of  $\frac{a}{\sqrt{T_2 M_o}}$  given by Equation (16) for a value of  $n$ .

For the polynomial solutions to the Hermite differential Equation

$$\frac{d^2 F}{dU^2} - 2U \frac{dF}{dU} + 2nF = 0, \tag{18}$$

the correspondence eigen function

$$M_{yn}(U) = A_n e^{-\frac{U^2}{2}} F_n(U) \tag{19}$$

will always have the acceptable behaviour of going to zero as  $|U| \rightarrow \infty$ . This is true because, for large value of  $|U|$ , the exponential  $e^{-\frac{U^2}{2}}$  varies so rapidly than  $F_n(U)$  and completely dominates the behaviour of the eigen function. The polynomials  $F_n(U)$  are given according to the Rodrigues formula for the well defined Hermite differential Equation:

$$F_n(U) = (-1)^n e^{U^2} \frac{d^n}{dU^2} (e^{-U^2}) \tag{20}$$

From Equations (7) and (16), we can write

$$a = \left(\frac{U}{P}\right)^2 \frac{1}{\sqrt{T_2 M_o}} = \vartheta \sqrt{T_2 M_o} = \sqrt{T_2 M_o} (2n + 1) \tag{21}$$

Equation (21) shows that an acceptable solution of equation (6) can only be obtained if  $a$ , has certain discrete values.

In a porous system with a given value of  $\frac{a}{\sqrt{T_2 M_o}}$ , the direc-

tion of the positive constant  $a$ , can only take on one of  $\vartheta = (2n+1)$  possible values. The splitting of a state into different components is therefore a consequence of the difference values of  $a$ , arising from these directions in the porous medium. It is of great interest to note that the lowest allowed value of  $a$ , with  $n = 0$  in Equation (21) is not zero. This implies that, even in a very complicated porous medium, the lowest allowed value of  $a$ , always has a  $T_2$  relaxation parameter. This

is valid both in classical and quantum mechanical analysis of porous media.

**Variation of Porosity with Depth for Exploration Evaluation**

For exploration evaluations, we solved Equation (4a) when  $A = 0$  and arrived at a final solution:

$$P(x) = P_o e^{-kx} \tag{22a}$$

where  $P_o$  is the surface porosity,  $x$  is depth (m) and  $k$  is the compaction coefficient( $m^{-1}$ ).

$$k = \frac{T_o}{V} \tag{22b}$$

and

$$T_o = \frac{1}{T_1} + \frac{1}{T_2} \tag{22c}$$

Equation (22) relates the porosity with depth of burial. This type of analysis however will ignore the effect of varying overpressure between samples used to calibrate the function to a specific data set. In addition to relating the porosity with depth, Equation (22) can yield information on the dynamics of various parts of the porous medium. This involves measuring relaxation times such as  $T_1$  and  $T_2$  to determine other parameters such as correlation times, compaction coefficients, and chemical exchange rates. NMR relaxation is a consequence of local fluctuating magnetic fields within a molecule. Local fluctuating magnetic fields are generated by molecular motions. In this way, measurements of relaxation times can provide information of motions within a molecule on the atomic level. From Equation (22), the compaction coefficient has a reciprocal relationship with the fluid velocity.

**Quantum Mechanical Analysis of Porous Media**

The essential information in a porous medium which can be provided by a typical NMR experiment is the size distribution of fluid-field pores. The sizes of these pores are actually the basis for the classification of porous media; the microporous, the macroporous and the mesoporous (where we have the nanoporous materials). All these materials have their diameters in nanoscale (for the macroporous materials, diameter  $\geq 50nm$ ). It is expected that any fluid particle moving within these pores must definitely have its size quite smaller than the diameter of the pores. Such a size indicates that the fluid particle must behave like micro particles and hence, we need to treat the fluid particles inside the pores quantum mechanically. Equations (19) and (20) can be written in quantum mechanical form as

$$M_{yn}(P) = \left[ \frac{\sqrt[4]{\mu T_2 M_o}}{2^n n! \sqrt{\pi \hbar}} \right]^{1/2} \exp(-P^2 \frac{\sqrt{\mu T_2 M_o}}{2\hbar}) F_n(P) \tag{23}$$

$$F_n(P) = (-1)^n \exp(\frac{\sqrt{\mu T_2 M_o}}{\hbar} P^2) \frac{\hbar^{n/2}}{(\sqrt{\mu T_2 M_o})^{n/4}} \frac{d^n}{dP^2} \exp(-\frac{\sqrt{\mu T_2 M_o}}{\hbar} P^2) \tag{24}$$

where

$$a^2 = \frac{\mu}{\hbar^2} \tag{25}$$

$$A_n = \left[ \frac{\sqrt[4]{\mu T_2 M_o}}{2^n n! \sqrt{\pi \hbar}} \right]^{1/2} \tag{26}$$

The term  $\frac{\hbar^{n/2}}{(\sqrt{\mu T_2 M_o})^{n/4}}$  has been introduced such that

the function  $F_n(P)$  would behave quantum mechanically. From Equations (21) and (25) we derive

$$R_n = \left( \frac{1}{4T_{2n}} \right)^{1/2} = \frac{1}{2} \sqrt{R_{2n}} = \hbar \sqrt{\frac{M_o}{\mu}} \left( n + \frac{1}{2} \right) \tag{27}$$

$R_n$  are the transverse relaxation rate eigenvalues of the porous medium expressed in terms of the equilibrium magnetization  $M_o$ , mass  $\mu$ , of fluid particles inside the pore, the Planks constant  $\hbar$  and the quantum number  $n$ , for the porous medium. The quantum number determines the specific porous state which the fluid particles occupy within the pore. The state, and therefore spin-spin relaxation rate are quantized. They can be determined by the quantum number  $n$  which is any integer greater than or equal to zero. The graphics of Equation (23) are shown in Fig. (1) for  $n = 0, 1$ . From Equation (4b) the expression for the kinetic energy of fluid particles within the pore is obtained in Equation (28).

$$\frac{1}{2} \mu V^2 = \frac{\hbar^2}{2T_1 T_2} \times \frac{x^2}{P^2} \tag{28a}$$

or

$$\varepsilon = \left( \frac{x^2}{V^2 T_1} \right)^2 = a^4 T_2^2 P^4 = \frac{\mu^2}{\hbar^4} T_2^2 P^4 \tag{28b}$$

From Equations (21) and (28b), we can write

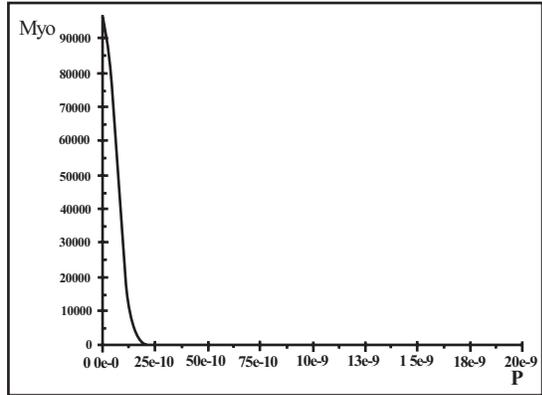
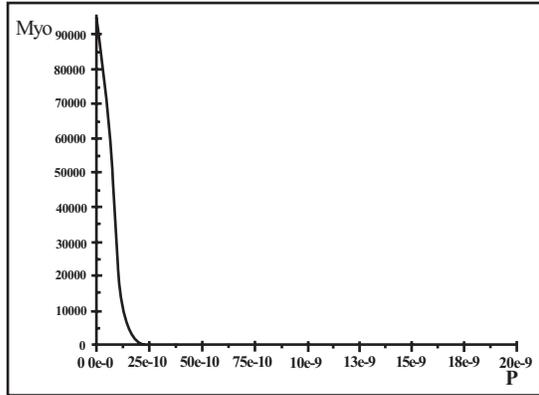
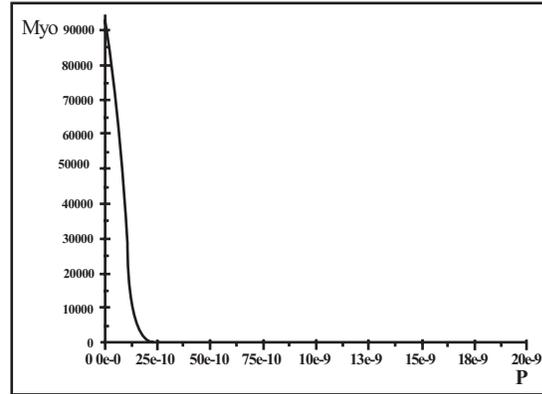
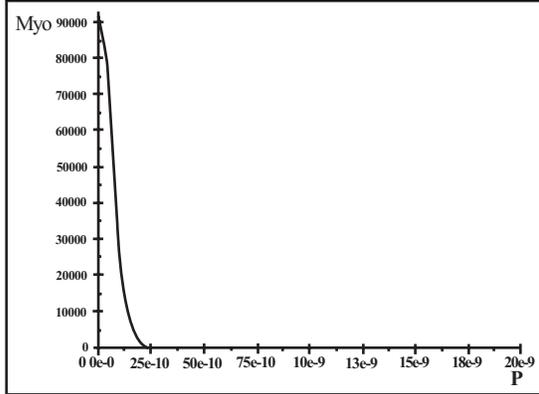
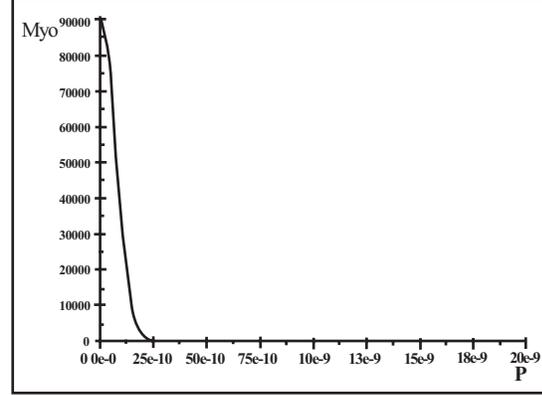
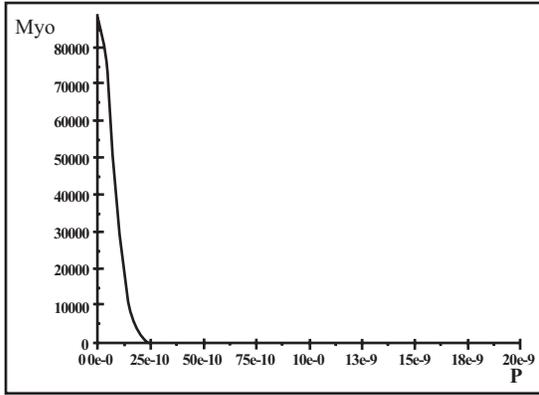
$$V = \frac{x}{P \sqrt{T_2 T_1} \sqrt{T_2 M_o} (2n + 1)} \tag{28c}$$

The quantity  $\varepsilon$ , is a very important parameter derived from the relationship between NMR porosity and  $T_2$  relaxation time. The graphics of equations (28a) are shown in Fig. (2).

The application of Darcy's law is the standard approach to characterize single phase fluid flow in microscopically disordered and macroscopically homogeneous porous media [28-30]. Basically, one simply assumes that a global index, the permeability  $k$ , relates the average fluid velocity  $V$ , through the pores, with the pressure drop  $\Delta p_f$  measured across the system as,

$$V = -\frac{k}{\eta} \frac{\Delta p_f}{L} \tag{28d}$$

(a)



(b)

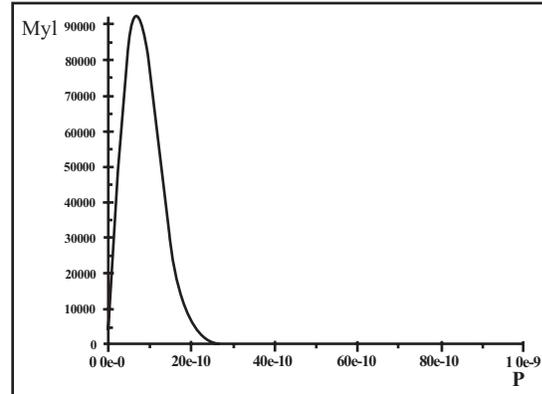
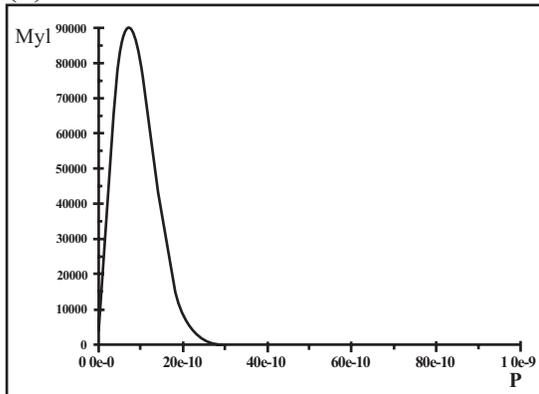


Fig. (1). Contd.....

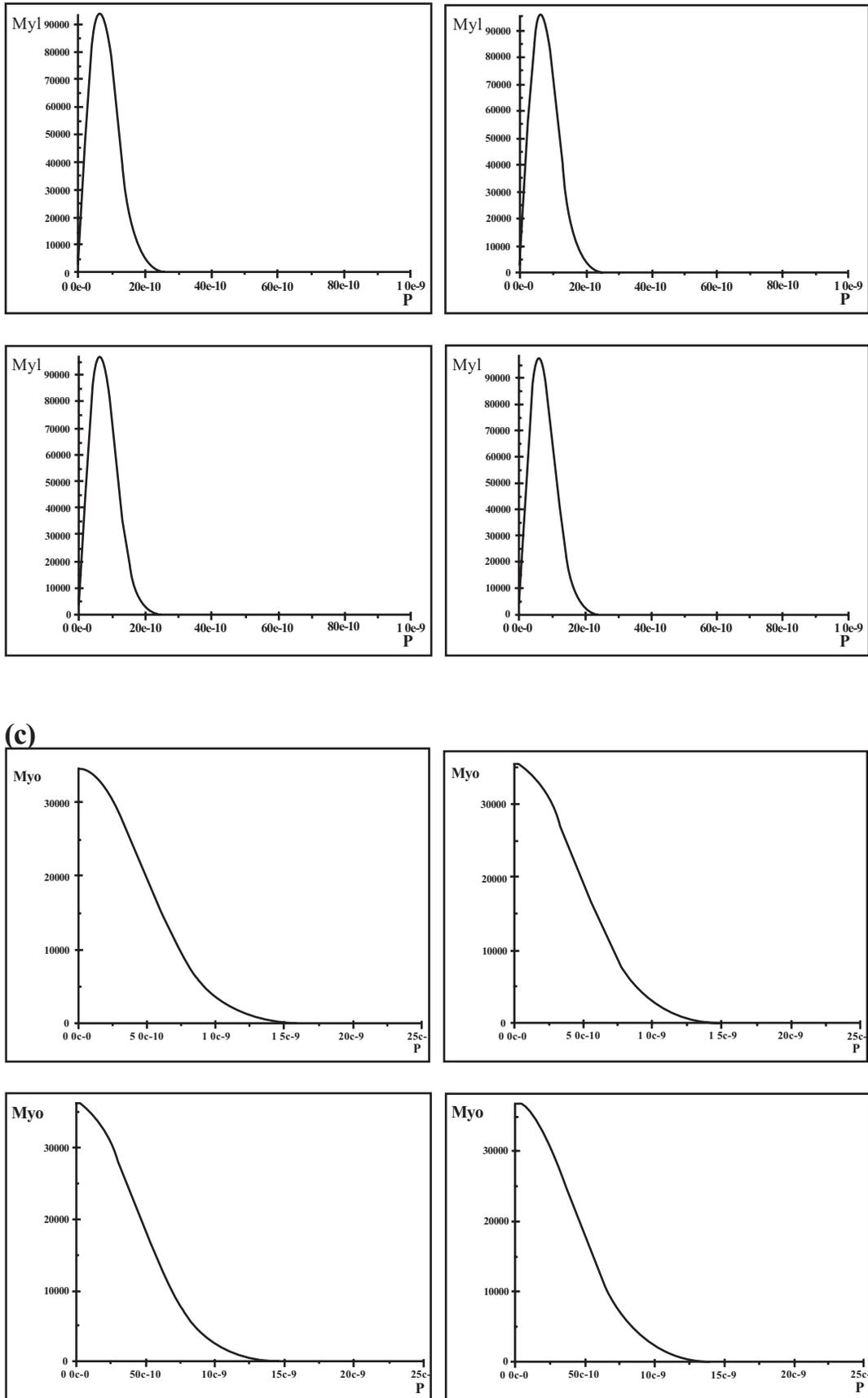
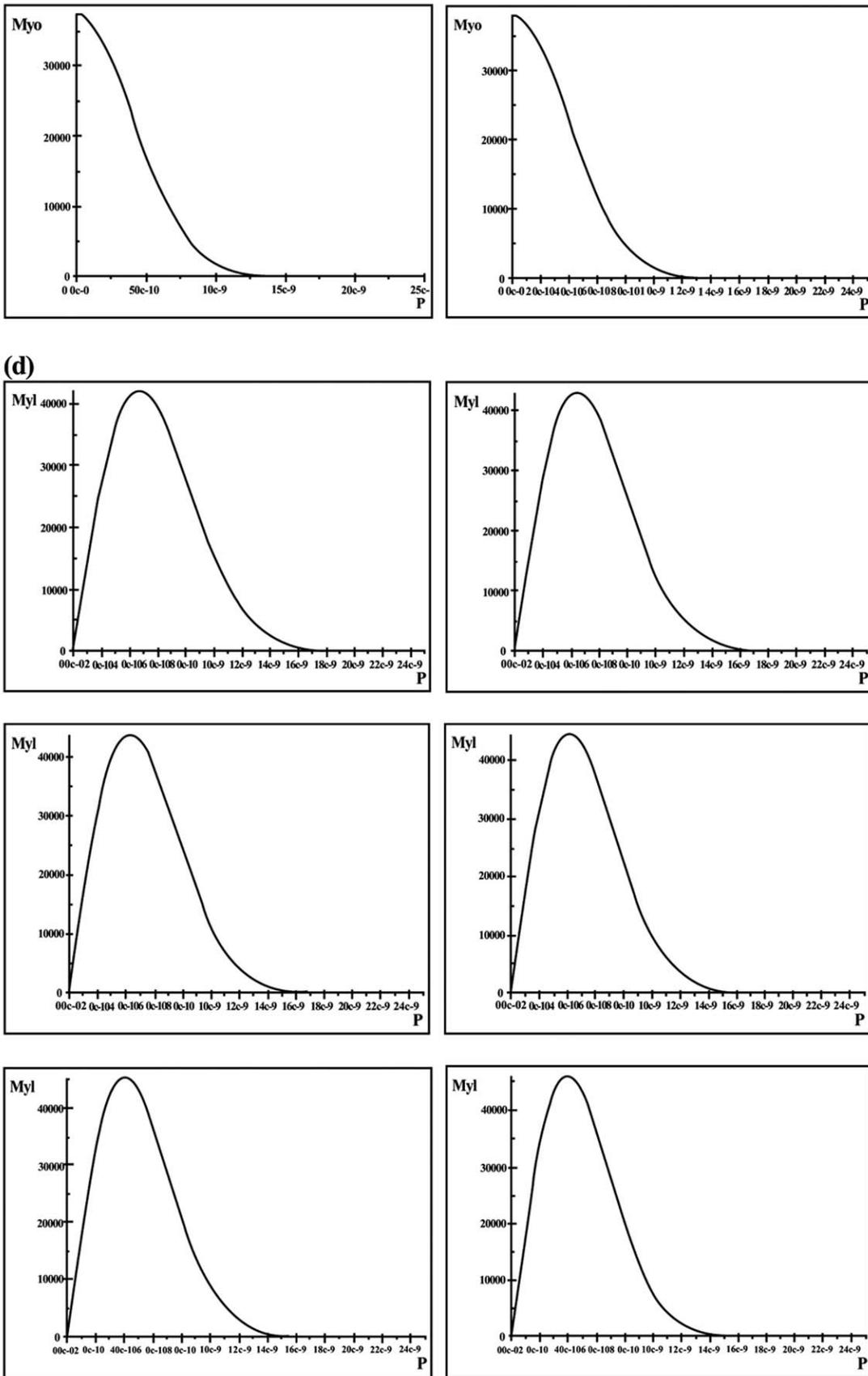


Fig. (1). Contd.....



**Fig. (1).** Graphics of equations (23&24) for proton (a)  $n = 0$ , (b)  $n = 1$ ; electron (c)  $n = 0$  (d)  $n = 1$  for the values of  $T_2 = 0.25s, 0.3s, 0.35s, 0.4s, 0.45s, 0.5s$ .

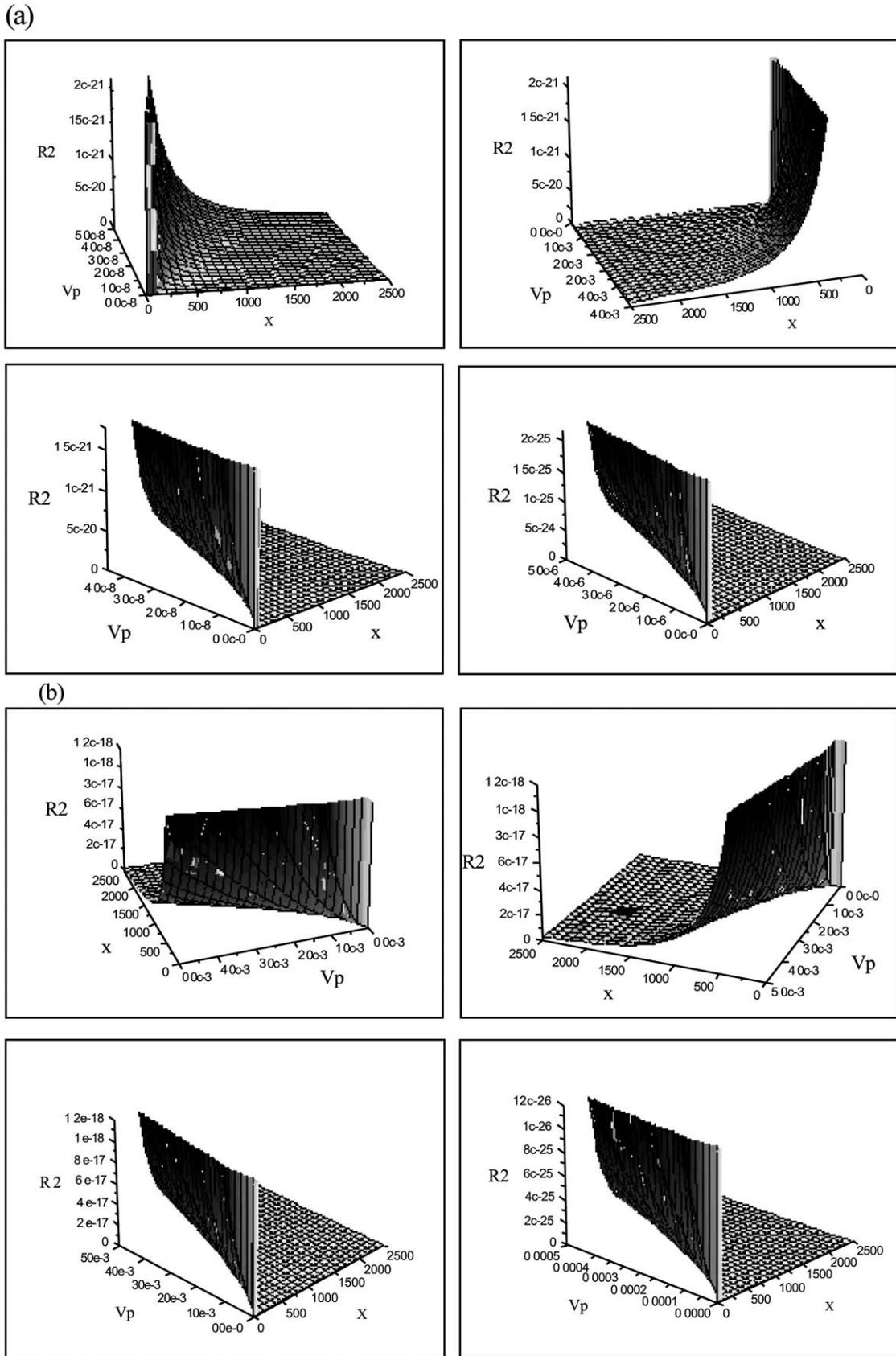


Fig. (2). Graphics of equation (28a) for (a) proton and (b) electron when  $T_1 = 1$ .

where  $L$  is the length of the sample in the flow direction and  $\eta$  is the viscosity of the fluid. However, in order to understand the interplay between porous structure and fluid flow, it is necessary to examine local aspects of the pore space morphology and relate them with the relevant mechanisms of momentum transfer (viscous and inertial forces). Previous studies [31-33] where computational simulations based on the knowledge of the pore space morphology were quite successful in predicting permeability coefficients of real porous materials. From Equation (28c and 28d), we can write an expression for the flow velocity as

$$V = \frac{x}{P\sqrt{T_2T_1}\sqrt{T_2M_o}(2n+1)} = -\frac{k}{\eta} \frac{\Delta p_f}{L} \quad (28e)$$

### NMR Relaxation Mechanism

There are three NMR relaxation mechanisms that influence  $T_1$  or  $T_2$  relaxation time within a pore: grain surface relaxation, relaxation by molecular diffusion in magnetic field gradients and relaxation by bulk fluid processes. For a single pore, the nuclear spin magnetization decays exponentially and the signal amplitude of time in a  $T_2$  experiment decays with characteristic time constant  $(\rho_2 \frac{s}{\Omega})^{-1}$ . Therefore,

we can write

$$\frac{1}{T_1} = (\rho_1 \frac{s}{\Omega}) \quad (29a)$$

and

$$\frac{1}{T_2} = (\rho_2 \frac{s}{\Omega}) \quad (29b)$$

where  $\rho_1$  and  $\rho_2$  are  $T_1$  and  $T_2$  surface relativities at surface  $s$ , respectively and  $\Omega$  is the volume of the pore. Porous media have a distribution of pore sizes, each with its own value of  $s/\Omega$ . The total magnetization is the sum of the signal coming from each pore. The sum of the volumes of all the pores is equal to the fluid volume of the media-the porosity. The total signal is therefore proportional to porosity and the overall decay is the sum of the individual decay which reflects pore size distribution, one of the key elements of NMR interpretation. From equations (28, 29), we derive

$$x^2 d_e^2 = \frac{\rho_1 \rho_2 \mu s^2 \hbar^2}{V^2 \Omega^4} \times \frac{x^4}{P^2} \quad (30)$$

where

$$d_e = \frac{\mu}{\Omega} \quad (31)$$

is the density of fluid particle. If we assume that  $x$  is the depth of the fluid particle (or its height below the surface), then  $dgx$  gives the pressure on the fluid particle  $p_f$ . Equation (30) gives

$$p_f = \frac{\sqrt{\mu \rho_1 \rho_2}}{P} \left( \frac{sg\hbar}{V} \right) \left( \frac{x}{\Omega} \right)^2 \quad (32)$$

where

- $p_f$  = pressure on the fluid particle
- $\mu$  = mass of the fluid particle
- $\rho_1$  = relaxivity associated with the  $T_1$  relaxation time
- $\rho_2$  = relaxivity associated with the  $T_2$  relaxation time
- $s$  = surface area of the fluid pore
- $V$  = fluid flow velocity
- $G$  = acceleration due to gravity
- $\hbar = \frac{h}{2\pi}$  = Plank's constant
- $\Omega$  = volume of the fluid in the pore
- $P$  = porosity
- $x$  = height of the pore below the surface

Equation (32) accurately relates the required parameters involved in poromechanics.

### CONCLUSION

We have presented a classical and quantum mechanical method of solving the Bloch NMR flow equations to study qualitatively, two of the most important parameters (permeability and porosity) used to characterize porous media. The mathematical formulation for the first time establishes a method that allows for simultaneous measurement of permeability, porosity, pore size distribution of a core, pressure gradient and the depth of the pore in terms of NMR parameters. This is very significant because, the pore size distribution can be determined noninvasively and can be observed simultaneously under varying pressure with other experiments such as the permeability measurement. Additionally, NMR makes use of the intrinsic property of an atom in which when a radio frequency wave is applied to the substance containing the atom, a signal is produced carrying a wealth of information about the particular particle(s) present and the surroundings. That is, whenever we apply the RF wave to the fluid particle within the pore, we get signal (the transverse magnetization) carrying information on the nature of the fluid and the pore which is its surrounding.

It is particularly observed that Equation (32) accurately relates the parameters involved in poromechanics. As the pressure increases, the porosity decreases and so is the fluid velocity and the pore volume. At the same time, the relaxation times become relatively long. This accurately agrees with experiment. Since the pores are actually meant for some particles (fluid particles) to flow from one point to the other, accurate understanding of these particles and their motion as formulated in this study, can reveal significant information about the porosity and other important properties of the pore. It is quite interesting that accurate understanding of the pore properties can also reveal the chemical composition of the fluid within the pore. This knowledge could be very crucial in the design of better gas masks.

In spite of its great applicability, the concept of permeability as a global index for flow, which implies the validity of Equation (28e), should be restricted to viscous flow conditions or, more precisely, to values of the Reynolds number,

$$Re = \frac{dVr_p}{\eta} \quad (33a)$$

where  $d$  is the density of the fluid and  $r_p$  is the grain diameter. From Equations (28c and 30), equation (33) becomes

$$Re = \frac{\sqrt{\rho_1 \rho_2 \mu s \hbar} x Vr_p}{V\Omega^2 P \eta} \quad (33b)$$

or

$$Re = \frac{x}{P\sqrt{T_2 T_1} \sqrt{T_2 M_o} (2n+1)} \frac{r_p d}{\eta} \quad (33c)$$

Since porous materials are either microporous (pore diameter smaller than 2nm), macroporous (pore diameter greater than 50nm) or mesoporous (pore diameter greater than 2nm and less than 50nm), the analytical expressions showing the direct relationship between the pore features and the NMR parameters obtained in this presentation can make our adventure into porous media quite exciting, motivating and rewarding.

The polynomials for the NMR transverse magnetization are obtained in Equation (23) where  $F_n(P)$  is the Hermite polynomials and satisfies Equation (18). The generating functions and recurrence relations of the Hermite polynomials can be invaluable tools for the analysis of fluid flow in porous media. Specifically, if we assume an rF-pulse of the form

$$\gamma B_1(x) \approx \sin(x/l) \quad \text{where } 0 < l < x \quad (34a)$$

The NMR transverse magnetization in the porous media based on Equations (5 and 22) become a simple experimental value

$$M_y(P) = \frac{\sin(x/l)}{P_o^2} e^{2\frac{T_o}{V}x} \quad \text{where } 0 < l < x \quad (34b)$$

This simplification can represent a mathematical tool for future experimental procedure.

Based on Equation (5), it can be very informative to note that Equation (6) or (8) is the Schrödinger equation in terms of dimensionless kinetic energy defined by

$$t(U) = \zeta - U^2 \quad (35a)$$

where the positive constant  $a^2$  is chosen such that

$$\frac{a}{\sqrt{M_o T_2}} = \zeta \quad (35b)$$

In Equation (35),  $\zeta$  is a dimensionless quantity. The computational analysis of Equation (35a) and some of its

applications have been demonstrated for  $\zeta = 1, 11,$  and  $39$  respectively [31]. The NMR transverse magnetization (NMR signal) shows clearly the general feature of harmonic oscillator wavefunctions, that the oscillations in NMR signal have the smallest amplitude and loop length near  $U = 0$ , where the kinetic energy is largest, and the largest amplitude and loop length near the classical turning points, where the kinetic energy is near zero [31].

Specifically, if we put  $a^2 = 1$  in Equation (6) the graphics of  $M_y(P)$  as a function of  $P$  for blood flow in a porous medium where  $T_2 = 0.5s$  and  $M_o = 2$ , is the same for

$\zeta = 1$  discussed above. Based on Equations (5 and 6), it would not be difficult to design appropriate rf  $B_1(x)$  field depending on the intrinsic NMR properties of the fluid in the pore.

The qualitative evaluation of porous media discussed in this study can be very important not only in the field of inorganic chemistry, oil and gas industry or medicine, but also in that of soil science. In fact, the application of the solutions suggested may have important implications also for the study of environmental matrices.

It can be very interesting to note that: 1) the results presented in Fig. (1), may apply to EPR under specific conditions of frequency, rf  $B_1(x)$  field, static magnetic field,  $T_1$  and  $T_2$  relaxation parameters. 2) at 50 nm it is believable that surface interactions as stated in Equation (29) are dominant. Will the surface interaction always be dominant for all possible liquids in all possible pore surfaces at all possible temperatures? These will be the focus of our next investigation.

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