

FORMULATION OF TIME DEPENDENT BLOCH NMR EQUATION FOR COMPUTATIONAL ANALYSES OF NANO PARTICLES IN POROUS MEDIA

ABSTRACT

Nuclear Magnetic Resonance (NMR) has been very useful in the study of pore size distribution of porous materials and in molecular recognition. Important properties of the porous media have been shown to be very much dependent on the T_1 and T_2 relaxation times. The NMR transverse magnetization carries information on the pores' properties. This has been demonstrated by many experiments on porous media but analytical expressions showing the direct relationships between the pore features and the NMR parameters have been quite scarce in literature. In this study, quantum mechanical formulation of time dependent Bloch NMR equation for computational analyses of nano particles in porous media has been presented. Since the nano particle is expected to be imaged in a nano-porous medium, we apply the transformation that makes the NMR transverse magnetization $M_y(t)$ expressible in term of $M_y(p)$ with porosity $p(t)$. Two new parameters which validate the transformation are properly defined in terms of the porosity, T_1 and T_2 relaxation parameters.

Keyword; Bloch NMR equations, quantum mechanics, porosity, Transverse magnetization, nano particles, Porous media.

INTRODUCTION

Magnetic Resonance Imaging technique for nano-particle in biological system is a multiphysics process involving diverse physical domains such as magnetic fields and fluid dynamics. It is also a multiscale process ranging from mini dimensions of the arteries to micro dimensions of the capillaries and micro particles down to the nano dimensions of single domain super paramagnetic particles [6, 7]. Evidently there is neither a complete modelling framework nor a single software package for simulating the entire process. This would require the integration of multiparticle simulation, molecular simulation, continuum-based models, stochastic methods and nanomechanics [1, 16]. Nonetheless, critical physical parameters are captured by the simplified model of the fundamental Bloch NMR flow equation specifically adopted for porous medium. The analytical solutions to the Bloch equation can provide fundamental computational tools which can stimulate interest for future research at the molecular and atomic scales for conceptualization, characterization, development of nano particles either in the form of nanorobots or nano machines [10, 2].

In this study, we have solved the time dependent modified Bloch NMR equations [3, 4, 5]:

$$\frac{d^2 M_y}{dt^2} + T_0 \frac{dM_y}{dt} + (T_g + \gamma^2 \beta^2_1(t)) M_y = \frac{M_0 \gamma \beta_1(t)}{T_1} \quad (1a)$$

Based on the condition: $\gamma^2 \beta^2_1(t) \ll \frac{1}{T_1 T_2}$

Where

$$\frac{1}{T_1 T_2} = T_g, \quad \frac{1}{T_1} + \frac{1}{T_2} = T_o$$

Equation (1a) becomes:

$$\frac{d^2 M_y}{dt^2} + T_0 \frac{dM_y}{dt} + T_g M_y = \frac{M_0 \gamma \beta_1(t)}{T_1} \quad (1b)$$

Equation (1a) can be solved based on three reasonable initial conditions:

1. $M_0 \neq M_z$; a situation which holds good in general and in particular when radio frequency $B_1(t)$ field is strong say of the order of 1.0 G or more.
2. Before entering the signal detector coil, nanoparticle bolus has magnetization $M_x=0$, $M_y=0$.
3. $B_1(t)$ is large; $B_1(t) \gg 1G$ or more so that M_y of the nanoparticle bolus changes appreciably from M_0 .

Equation (1b) can be significantly useful to analytically model the phenomenological dynamics of a nano particle moving through a biological porous material. Since the nano particle is expected to be imaged in a nano-porous medium (blood flow), we apply the transformation [3] that will make $M_y(t)$ expressible in term of $M_y(p)$. This condition transforms $M_y(t)$ into a porous medium with porosity $p(t)$, such that

$$\frac{dM_y}{dt} = \frac{dM_y}{dp} \frac{dp}{dt} \quad (2a)$$

Using the product rule, the second derivative can be derived:

$$\frac{d^2 M_y}{dt^2} = \frac{d^2 M_y}{dp^2} \left(\frac{dp}{dt} \right)^2 + \frac{dM_y}{dp} \frac{d^2 p}{dt^2} \quad (2b)$$

Equation (1a) becomes:

$$\frac{d^2 M_y}{dp^2} \left(\frac{dp}{dt} \right)^2 + \frac{dM_y}{dp} \frac{d^2 p}{dt^2} + T_0 \frac{dM_y}{dp} \frac{dp}{dt} + (T_g + \gamma^2 \beta_1^2(t)) M_y = \frac{M_0 \gamma \beta_1(t)}{T_1} \quad (3)$$

Equation (3) can be written in the form

$$\frac{d^2 M_y}{dp^2} + A \frac{dM_y}{dp} + a^2 M_y = a^2 T_2 M_0 \gamma \beta_1(t) \quad (4a)$$

where

$$A = \left[\frac{\left(\frac{d^2 p}{dt^2} \right)}{\left(\frac{dp}{dt} \right)^2} + T_0 \frac{\left(\frac{dp}{dt} \right)}{\left(\frac{dp}{dt} \right)^2} \right] \quad (4b)$$

$$a^2 = \frac{T_g}{\left(\frac{dp}{dt} \right)^2} \quad (4c)$$

For equation (4a) to be valid, parameter a^2 must be any positive integer and A must be a constant $p(t)$ is the porosity. For the purpose of obtaining fundamental (semi classical and quantum mechanical) information about the variation of porosity with time for fluid dynamics evaluation in porous media, we consider a case where A=0, equation (4a) becomes:

$$\frac{d^2 M_y}{dp^2} + a^2 M_y = a^2 T_2 M_0 \gamma \beta_1(t) \quad (5a)$$

Equation (5a) allows us to discuss the dynamics of the NMR system quantum mechanically if we define the radio frequency field as

$$\omega_1 = \gamma \beta_1(t) = P^2 M_y(p) << \frac{1}{\sqrt{T_1 T_2}} >> 1G \quad (5b)$$

Equation (5a) can be solved for the case of maximum signal where the equilibrium magnetization $M_0 = 0$ and when $M_0 \neq 0$.

SOLUTION OF THE BLOCH NMR FLOW EQUATION IN POROUS MEDIA

At maximum signal ($M_0 = 0$), equation (5) becomes

$$\frac{d^2 M_y}{dp^2} + a^2 M_y = 0 \quad (6)$$

The generalization solution to equation (6) when $a_1 = 0, a_0 \neq 0$, and all $a_{2n-1} = 0$ is given by:

$$M_{y1}(p) = (-1)^n c_0 \sum_{n=0}^{\infty} \frac{a^{2n} p^{2n}}{(2n)!} \quad (7)$$

When ($a_0 \neq 0, n = 2n-1, a_0 \neq 0$), the generalization solution to equation (6) is given by:

$$M_{y2}(p) = (-1)^n c_1 \sum_{n=1}^{\infty} \frac{p^{2n-1} a^{2(n-1)}}{(2n-1)!} \quad (8)$$

Equations (7) and (8) are the two fundamental solutions of equation (5) that is:

$$M_y(p) = (-1)^n c_0 \sum_{n=0}^{\infty} \frac{a^{2n} p^{2n}}{(2n)!} + (-1)^n c_1 \sum_{n=1}^{\infty} \frac{p^{2n-1} a^{2(n-1)}}{(2n-1)!} \quad (9)$$

Where $p = p(t) = p_0 \exp(-T_0 t)$

Solution to equation (5) for a physical case where the equilibrium magnetization $M_0 \neq 0$ leads to

Schrödinger wave equation for a simple harmonic oscillator and the Hermite differential equation:

$$\frac{d^2 M_y}{dp^2} + a^2 (1 - M_0 T_2 p^2) M_y = 0 \quad (10)$$

The solution to equation (10) is

$$M_{yn}(p) = H_n(p) \exp\left(-\frac{p^2}{2}\right) \quad (11)$$

where

$$H_n(p) = \sum_{n=0}^{\infty} C_n (T_2 M_o)^{\frac{1}{4}} a^{\frac{1}{2}} p(t) \quad (12)$$

and

$$2n+1 = \frac{a}{\sqrt{T_2 M_o}} \quad \text{Where } n=0, 1, 2, 3 \dots \quad (13)$$

Equation (11) becomes

$$M_{yn}(p) = \sum_{n=0}^{\infty} C_n (T_2 M_o)^{\frac{1}{4}} a^{\frac{1}{2}} p(t) \exp\left(-\frac{p^2}{2}\right) \quad (14)$$

We also derived a single valued solution of the Bloch NMR equation as

$$M_y(p) = D_1 \exp\left(\frac{(T_2 M_o)^{\frac{1}{2}} a p^2}{2}\right) \quad (15)$$

The general solution of equation (4b) when $A \neq 0$ is

$$p(t) = \frac{1}{A} \left\{ \ln[\exp(T_0 t)] - \ln[(K_2 \exp(T_0 t) - A)] \right\} + c_2 \quad (16)$$

VARIATION OF $M_y(p)$ WITH $P(t)$ AND TIME (s) FOR VARYING VALUES OF n

WHEN $M_o=0$ AND $A=0$

Analysis of equation (9) shows that the porosity of a nano porous material varies exponentially with NMR signal and relaxation parameter T_o . This implies that at the molecular level, the porosity decreases at an exponential rate as time of measurement increases, starting from the intrinsic maximum porosity of the material at time $t=0$ i.e. $P(t)=P_o$ where P_o was chosen to be unity as shown in figures 1-11. A possible explanation for this decay is because of the free induction decay experienced by the MR signal (Transverse Magnetization) when the equilibrium

magnetization M_0 have been assumed to be equal to zero. This implies that the total magnetic field B_1 applied to the nanoporous material is totally converted into magnetic force that excites the proton near the pore of the material and when the B_1 field is withdrawn, the magnetic force come down to zero freely through an exponential decay that starts from the maximum excitation that the B_1 field was able to give to the nano porous material's pore.

A 3D plot of $M_y(p)$, $p(t)$ and time (s) was made to visualize the behaviour of the MR signal (Transverse Magnetization) as the pore open up or closes down with time, which signifies the time or point of initiation of the nanoparticle's movement through the nanopores and a point when the movement has been completed by varying the number of harmonics (which corresponds to the number of protons in the pore been imaged) present in the MR signal. It was observed that the wave signifying the nature of the movement of the pore was more predominant and significant when the quantum number of harmonics $n=1$, more so, porosity was also consistent which invariably implies the motion of the nanoparticle through the nanopore at that instant and at a main field of 1.5T is consistent. The contour graph was used to simulate contrast of the MR signal as the porosity changes with time i.e. $P(t)$ was plotted against $t(s)$, and the contrast shown represents the intensity of the MR signal (Transverse Magnetization). In other words, the Legend shows the distribution of MR signal strength as porosity changes with time. This goes a long way to give handful information on how clear and the nature of stratification of MR signals, as the pore open up and closes down with time, for varying number of harmonics, and it was observed that a clearer contrast and layer (strata) was formed when the number of harmonics $n=1,2,\dots,10$. This tells us that the MR signal carries better information about protons for which $n=1$ and above. Hence for the second time it can be concluded that the MR signal carries more information about intrinsic proton of nanopores, relative to which the imaging of a

nanoparticle is made. Also a characteristics pattern-less nature of the contour plot for $n=0$ implies that no MR signal emerges in the absence of excitation of proton. Finally, for $n=2$ and above, the behaviour of the MR signal alternates with alternating odd and even value of harmonic number 'n'.

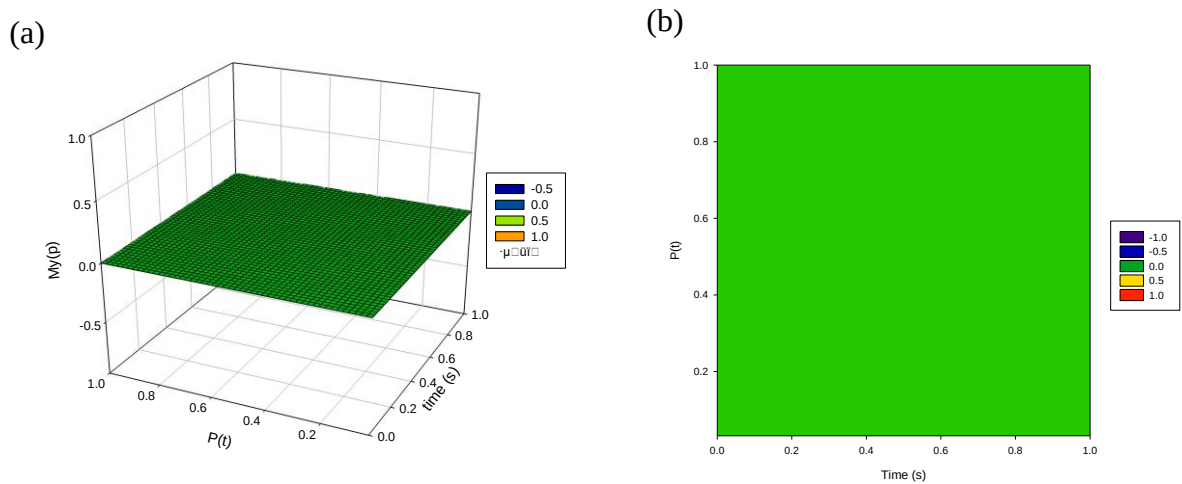


Fig 1: (a) 3 D graph of equation (9) for $M_0=0, A=0, n=0$ (b) Contour graph of equation (9) for $M_0=0, A=0, n=0$

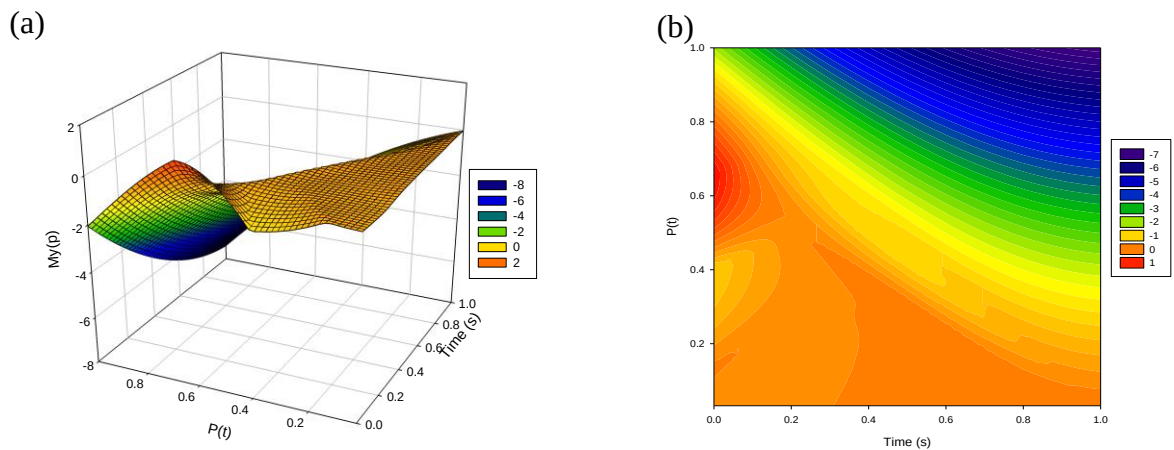


Fig 2: (a) 3 D graph of equation (9) for $M_0=0, A=0, n=1$ (b) Contour graph of equation (9) for $M_0=0, A=0, n=1$

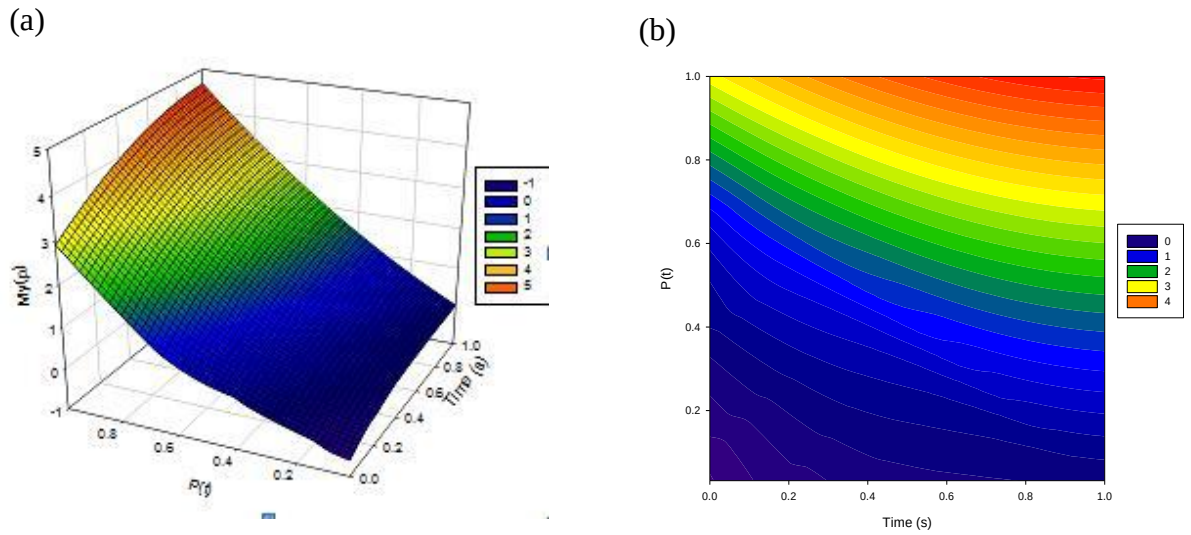


Fig 3: (a) 3 D graph of equation (9) for $M_o=0, A=0, n=2$ (b) Contour graph of equation (9) for $M_o=0, A=0, n=2$

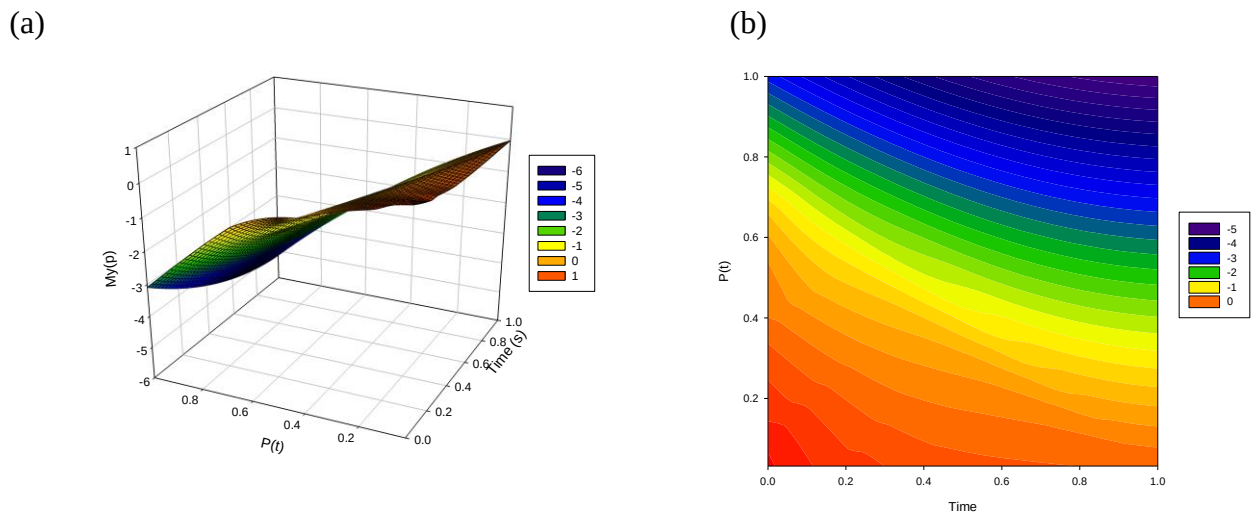


Fig 4: (a) 3 D graph of equation (9) for $M_o=0, A=0, n=3$ (b) Contour graph of equation (3.18b) for $M_o=0, A=0, n=3$

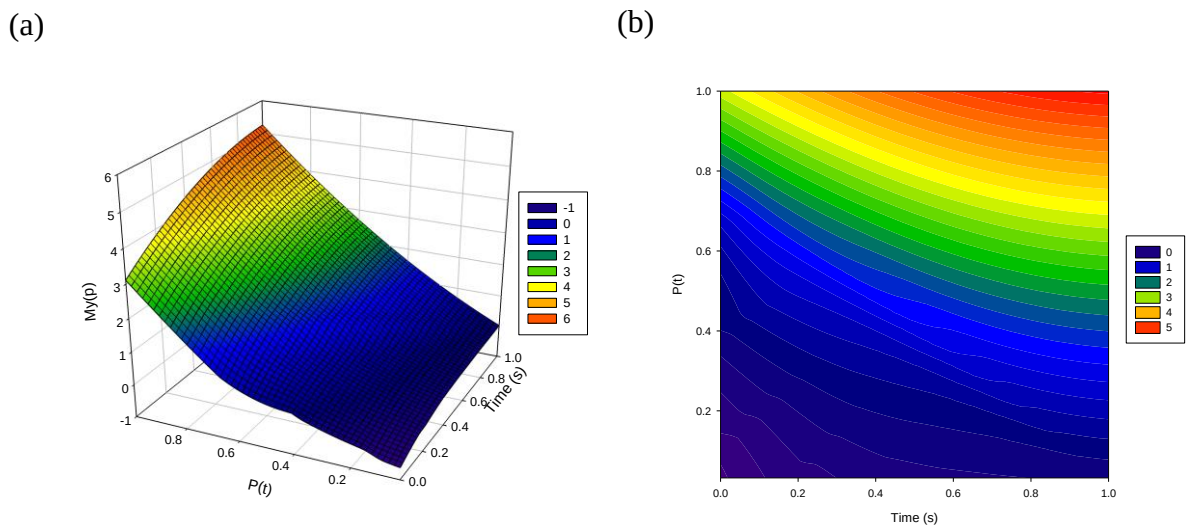


Fig 5: (a) 3 D graph of equation (9) for $M_o=0, A=0, n=4$ (b) Contour graph of equation (3.18b) for $M_o=0, A=0, n=4$

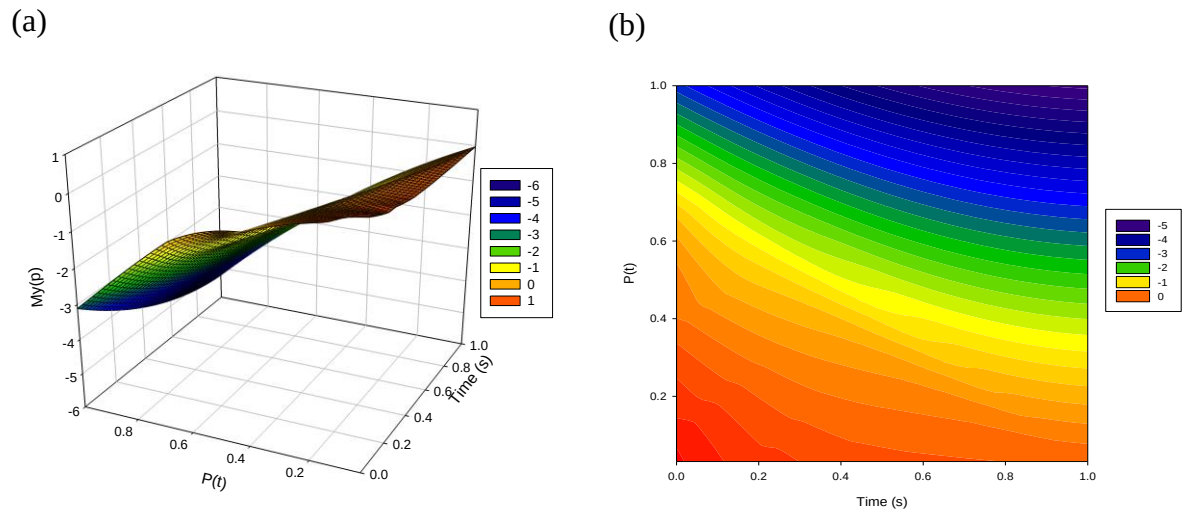


Fig6: (a) 3 D graph of equation (9) for $M_o=0, A=0, n=5$ (b) Contour graph of equation (9) for $M_o=0, A=0, n=5$

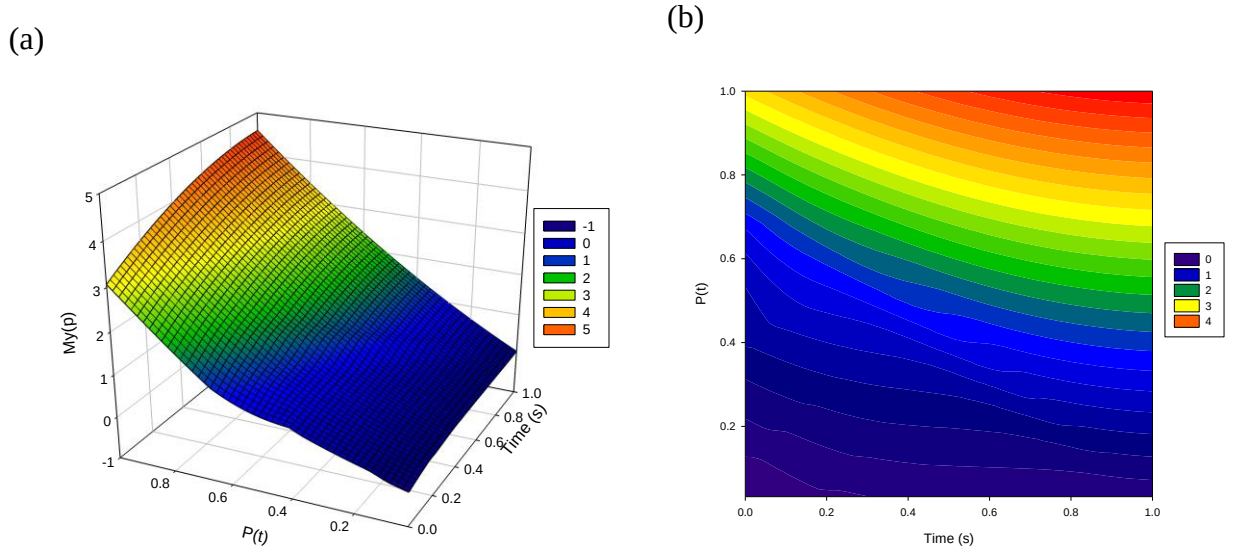


Fig 7: (a) 3 D graph of equation (9) for $M_o=0, A=0, n=6$ (b) Contour graph of equation (9) for $M_o=0, A=0, n=6$

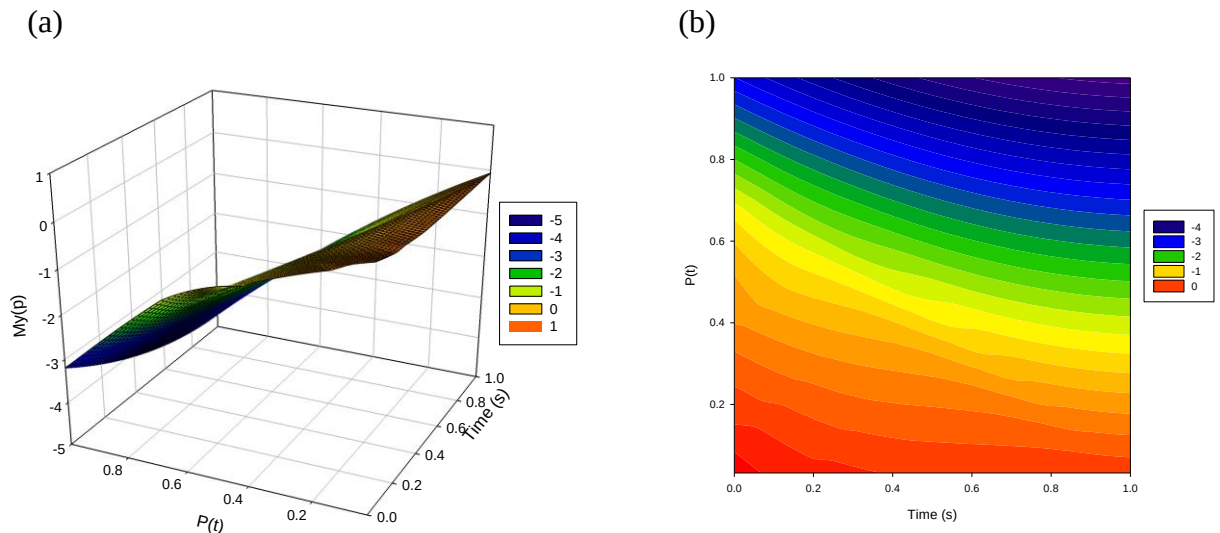


Fig 8: (a) 3 D graph of equation (9) for $M_o=0, A=0, n=7$ (b) Contour graph of equation (9b) for $M_o=0, A=0, n=7$

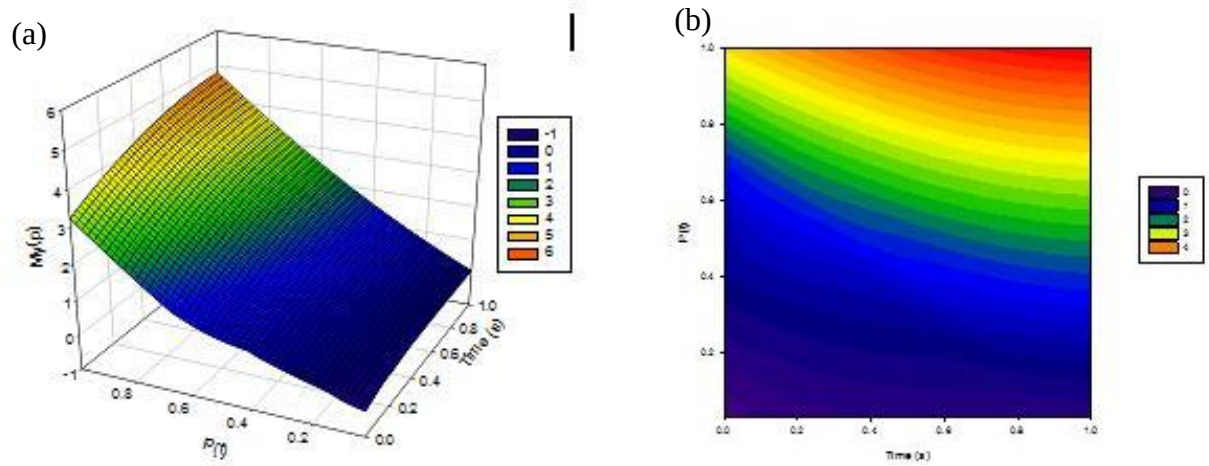


Fig 9: (a) 3 D graph of equation (9) for $Mo=0, A=0, n=8$ (b) Contour graph of equation (9) for $Mo=0, A=0, n=8$

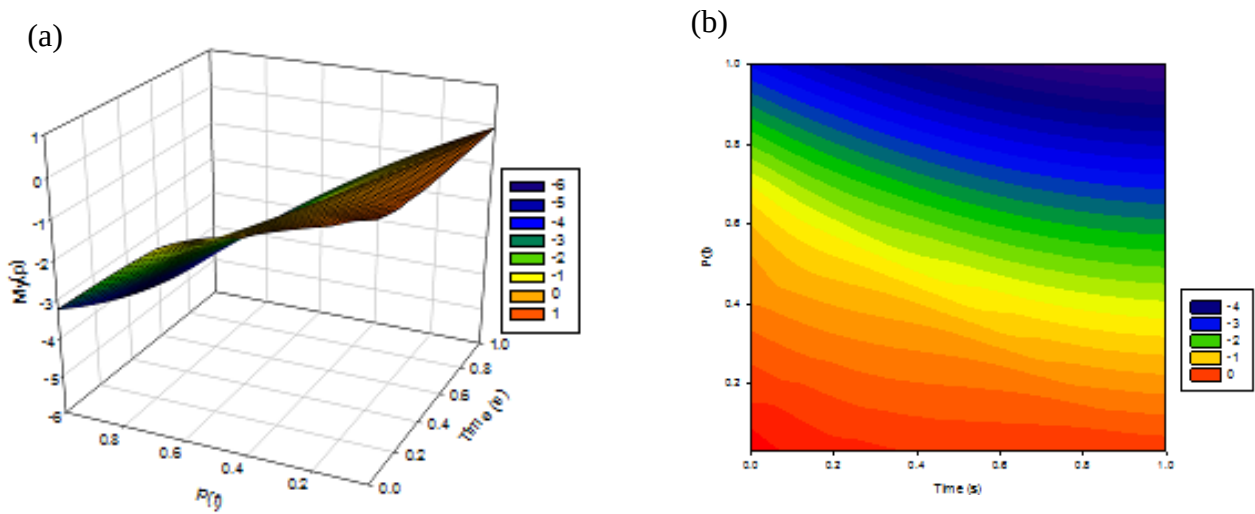


Fig 10: (a) 3 D graph of equation (9) for $Mo=0, A=0, n=9$ (b) Contour graph of equation (9) for $M_o=0, A=0, n=9$

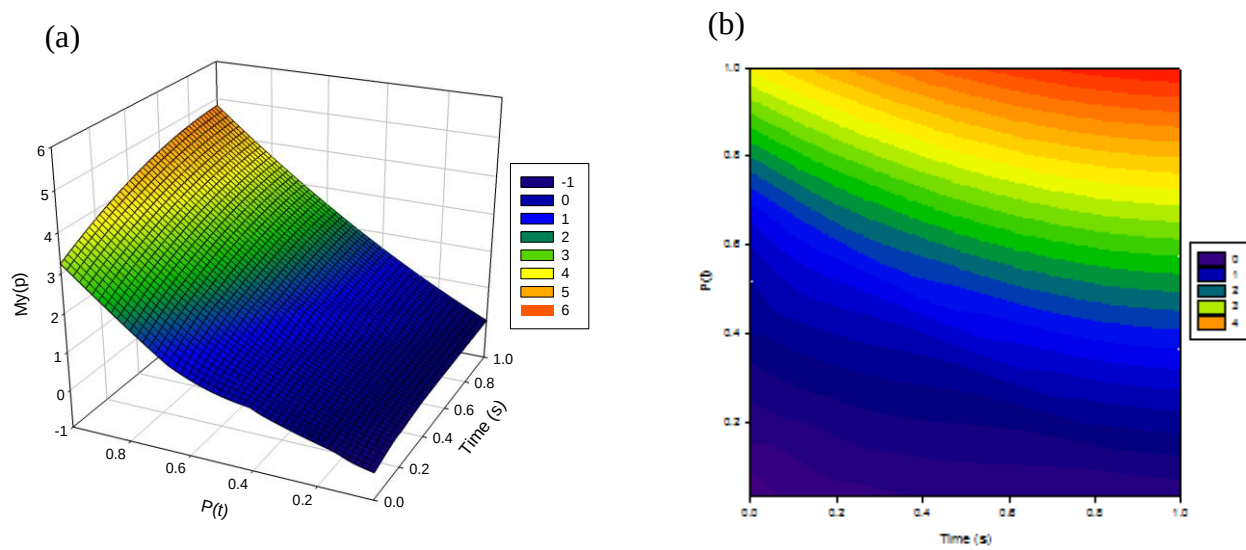


Fig 11: (a) 3 D graph of equation (9) for $Mo=0, A=0, n=10$ (b) Contour graph of equation (9) for $M_o=0, A=0, n=10$

VARIATION OF $M_y(p)$ WITH $P(t)$ AND $T(S)$ FOR VARYING VALUES OF n AND A WHEN $M_0 \neq 0$

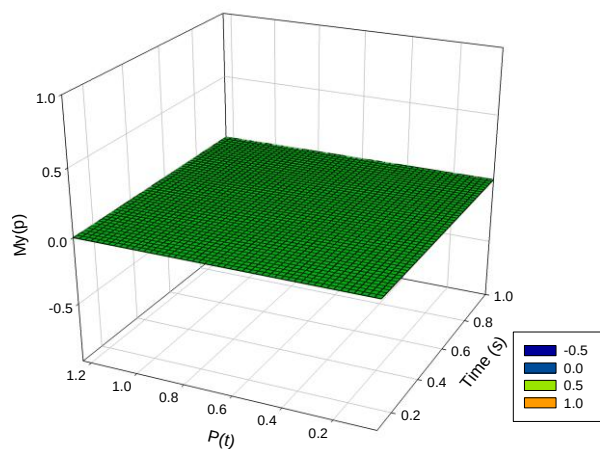
From a thorough characterization and vivid observation of figures 12- 16 that characterized equation (14), it was observed that for $n=0$ and $A=1$, there was no MR signal (Transverse Magnetization). This also shows that the transverse magnetization does not pick up as pore of nanoporous material opens or closes. Under this consideration, the porosity is not a pure exponential function of time, but a mixture of natural logarithm and exponential function of both the spin-lattice and spin-spin relaxation time. It was observed that as ‘ n ’ increases to 1, the behaviour of the MR signal changes and indicates that the pore is either opening or closing with time. The magnitude of MR signal increases slightly with time up to 0.6 sec after which the rate increases linearly. As ‘ n ’ increases to 2, the MR signal starts from a peak value for a single proton and decrease slowly with time up to 0.6 sec, where the signal start to decrease linearly. The MR signal maintain this trend as the pore opens with time until $n=4$ where the MR signal exhibit a full wave behaviour after a short ‘blankness’ for about 0.3 sec. As the pore opens towards its intrinsic porosity, the MR signal rapidly and linearly increases. The MR signal maintain the same trend even for $n=5$.

As ‘ A ’ increases to 2, the behaviour of MR signal generally is similar to that observed when A was equal to 1. Nonetheless, it is worthy of note that in some specific cases, some particular behaviours were observable, that include the fact that the full wave behaviour of MR signal slightly become less significant and that the magnitude of the MR signal become far and far greater than is observable when $A=1$. More so, it was observed that as ‘ A ’ increases, the maximum porosity of the pore found on a nanoporous material decreases. This implies that as ‘ A ’ increases, the maximum diameter with which the pore open up decreases. This is evident in

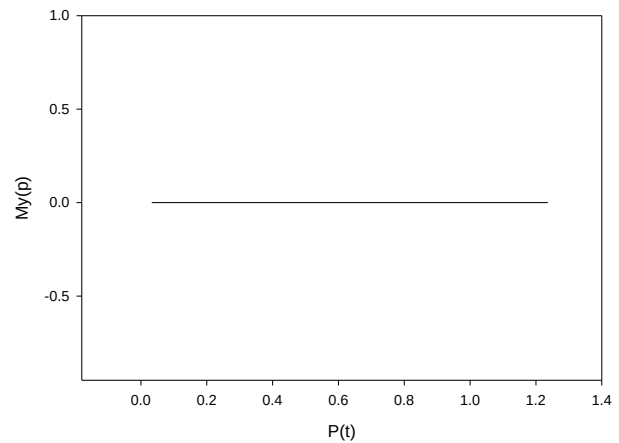
the solution given by equation (16), which gives no expression, about the surface's maximum porosity (otherwise known as the porous material's intrinsic porosity).

On a more broad term, it can be concluded based on the behaviour of these graphs that increase or decrease in the value of A only increases or decreases the maximum porosity observed respectively, which in turn increases the MR signal and make it behave similar to analysis given above as time of observation increases. Though there were exceptional cases where the MR signal decreases as in the case where quantum number 'n' equal 2 and 3.

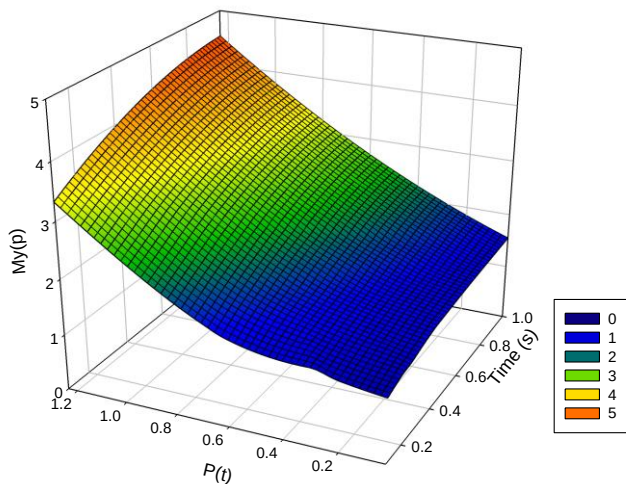
(a) 3D Graph of $My(p)$, $P(t)$ and $t(s)$ for $n=0$, $A=1$



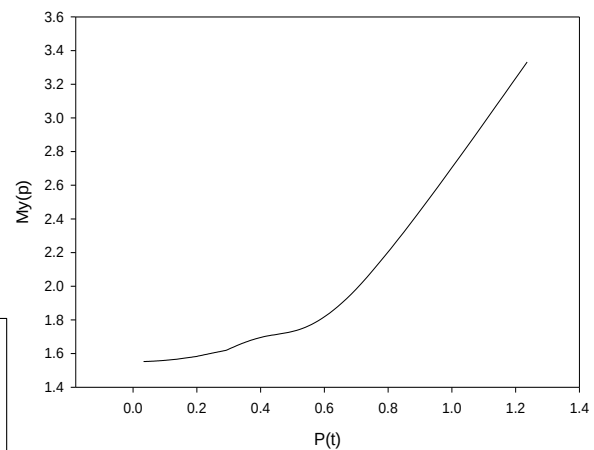
(b) 2D Graph of $My(p)$ and $P(t)$ for $n=0$, $A=1$



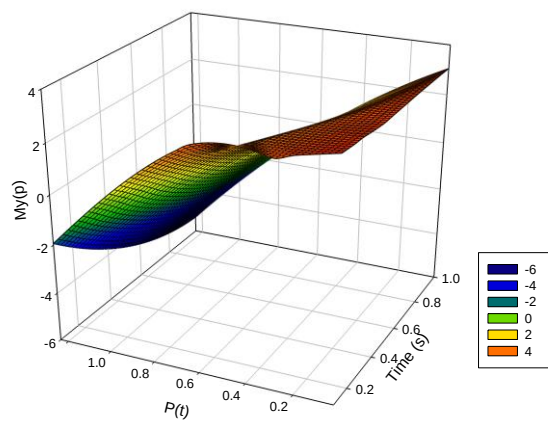
(c) 3D Graph of $My(p)$, $P(t)$ and $t(s)$ for $n=1$, $A=1$



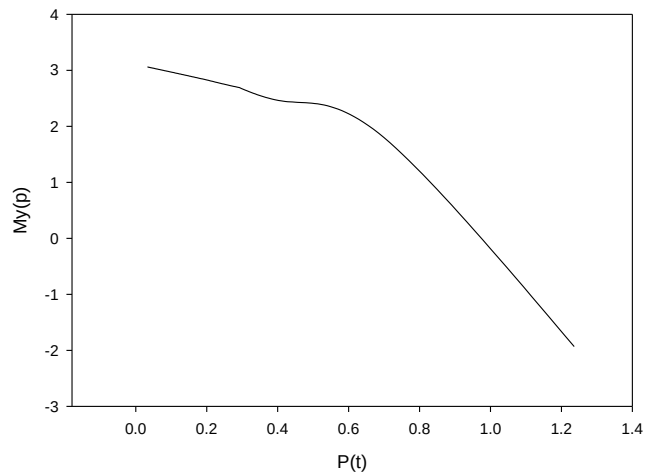
(d) 2D Graph of $My(p)$ and $P(t)$ for $n=1$, $A=1$



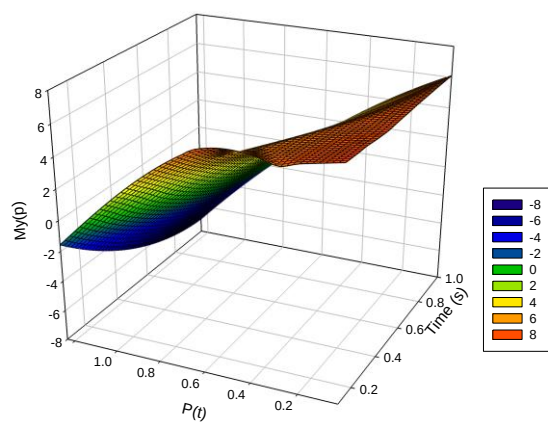
(e) 3D Graph of $My(p)$, $P(t)$ and $t(s)$ for $n=2$, $A=1$



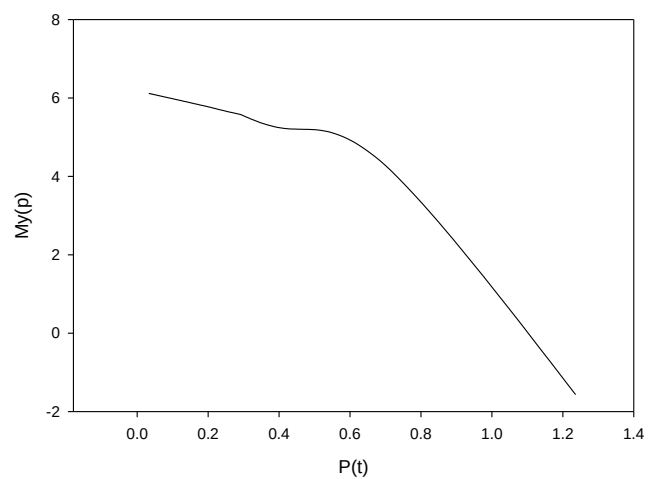
(f) 2D Graph of $My(p)$ and $P(t)$ for $n=2$, $A=1$



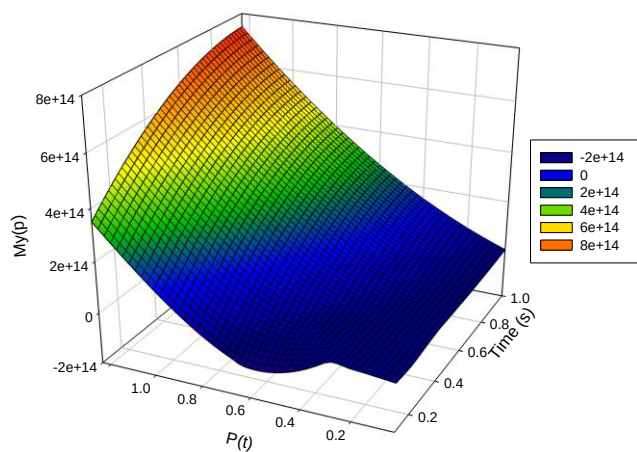
(g) 3D Graph of $My(p)$, $P(t)$ and $t(s)$ for $n=3$, $A=1$



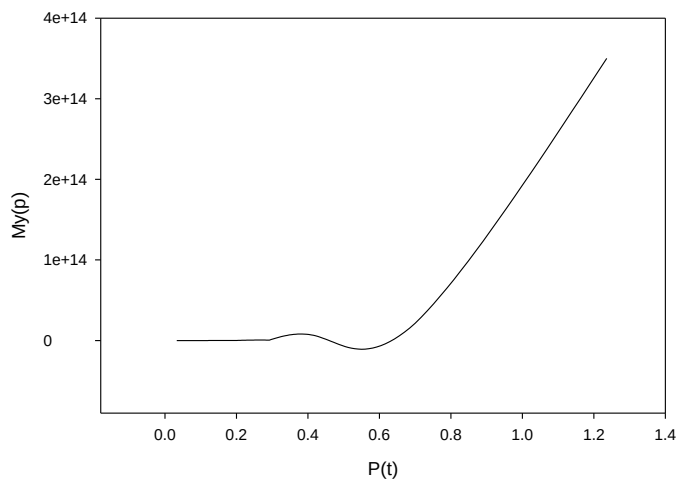
(h) 2D Graph of $My(p)$ and $P(t)$ for $n=3$, $A=1$



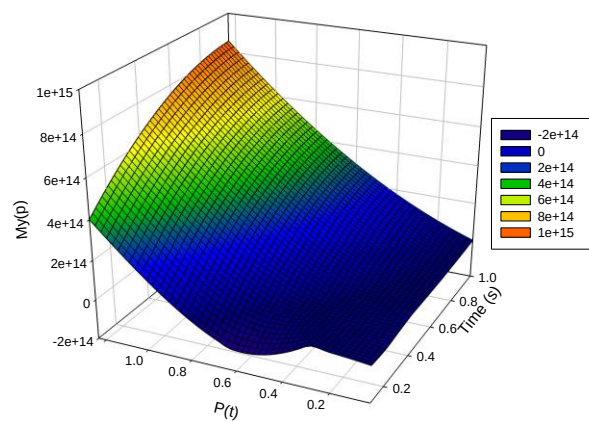
(i) 3D Graph of $My(p)$, $P(t)$ and $t(s)$ for $n=4$, $A=1$



(j) 2D Graph of $My(p)$ and $P(t)$ for $n=4$, $A=1$



(k) 3D Graph of $My(p)$, $P(t)$ and $t(s)$ for $n=5$, $A=1$



(l) 2D Graph of $My(p)$ and $P(t)$ for $n=5$, $A=1$

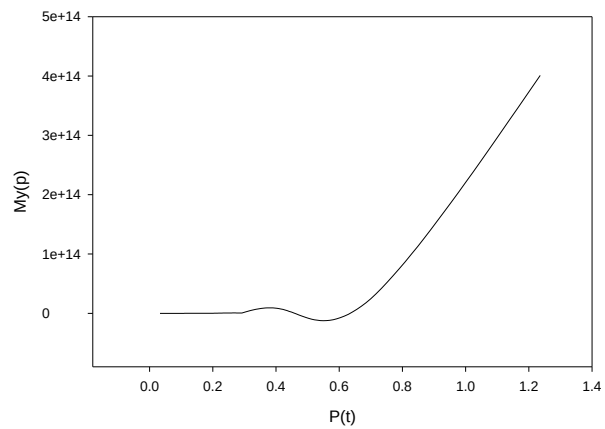
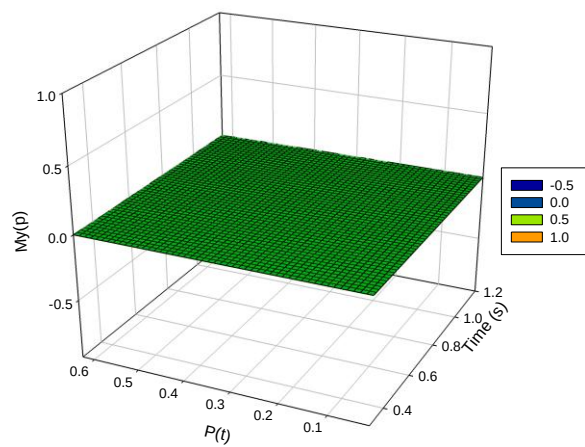
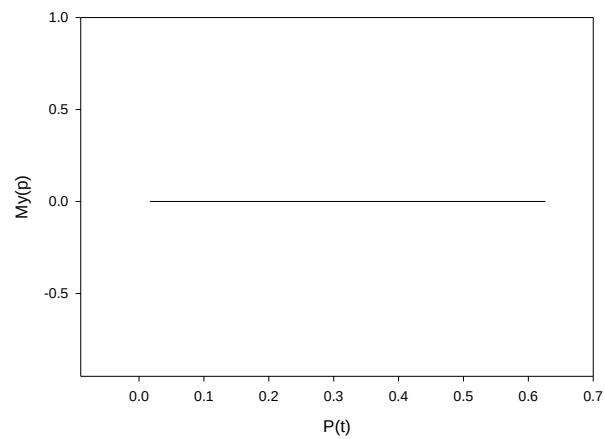


Fig 12: 3 D & 2 D graph of equation (14) for $A=1$, $M_o \neq 0$, (a) $n=0$ (b) $n=0$, (c) $n=1$, (d) $n=1$, (e) $n=2$, (f) $n=2$, (g) $n=3$, (h) $n=3$, (i) $n=4$, (j) $n=4$, (k) $n=5$, (l) $n=5$, for 3D and 2D respectively.

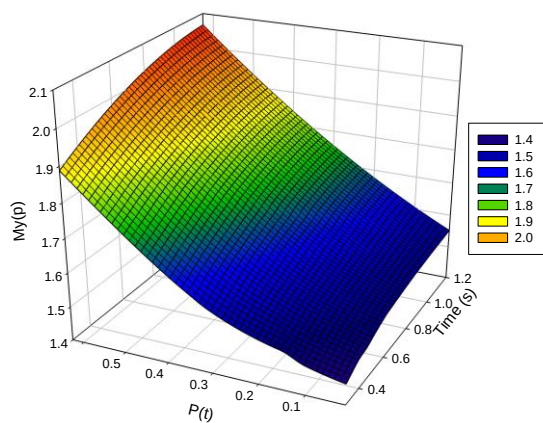
(a) 3D Graph of $My(p)$, $P(t)$ and $t(s)$ for $n=0$, $A=2$



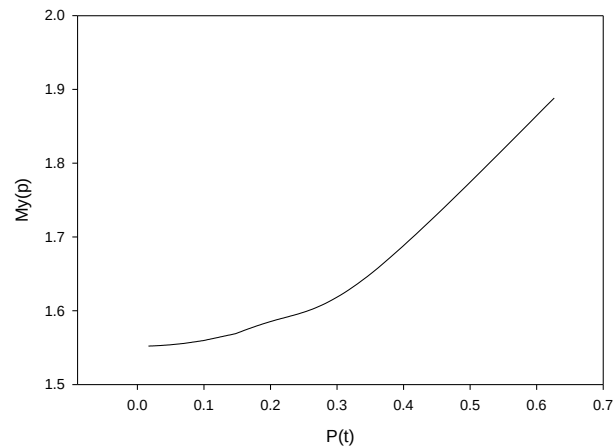
(b) 2D Graph of $My(p)$ and $P(t)$ for $n=0$, $A=2$



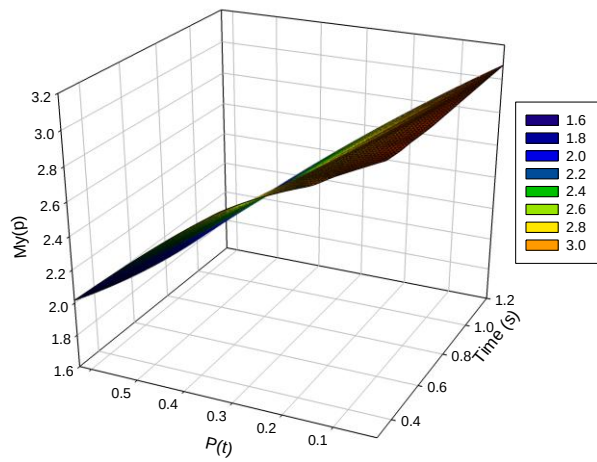
(c) 3D Graph of $My(p)$, $P(t)$ and $t(s)$ for $n=1$, $A=2$



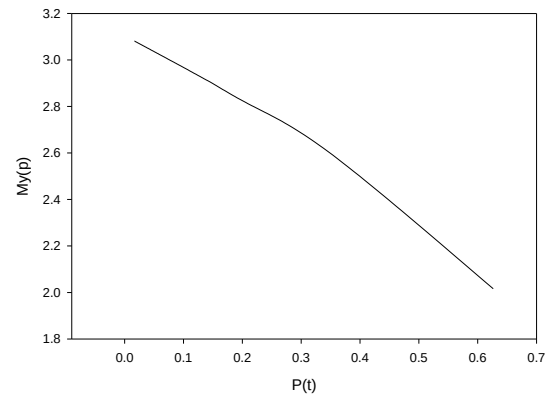
(d) 2D Graph of $My(p)$ and $P(t)$ for $n=1$, $A=2$



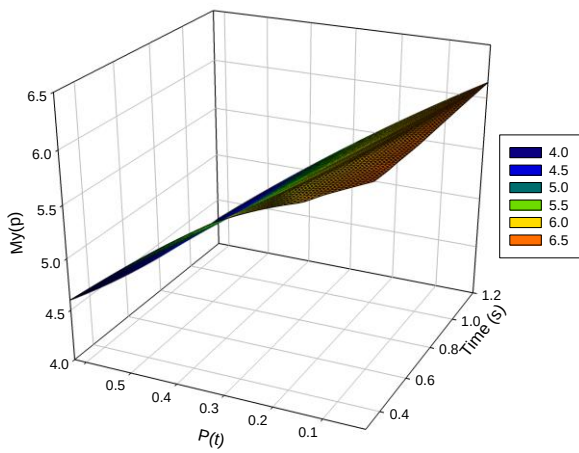
(e) 3D Graph of $My(p)$, $P(t)$ and $t(s)$ for $n=2$, $A=2$



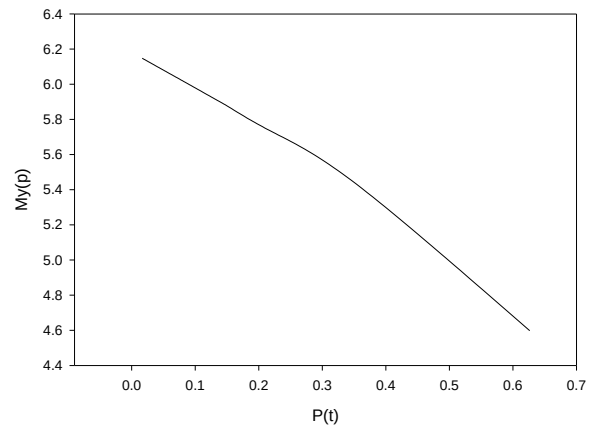
(f) 2D Graph of $My(p)$ and $P(t)$ for $n=2$, $A=2$



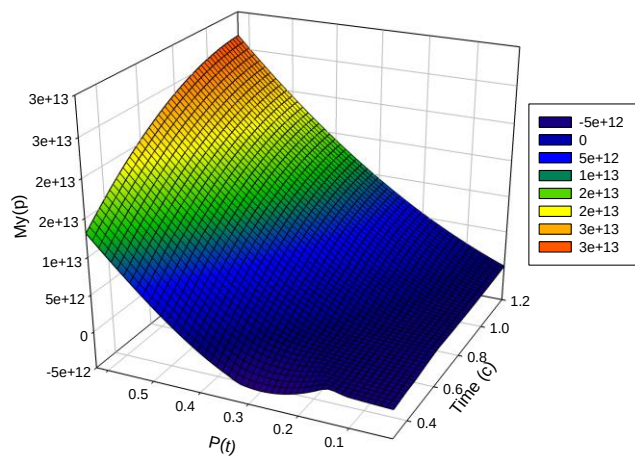
(g) 3D Graph of $My(p)$, $P(t)$ and $t(s)$ for $n=3$, $A=2$



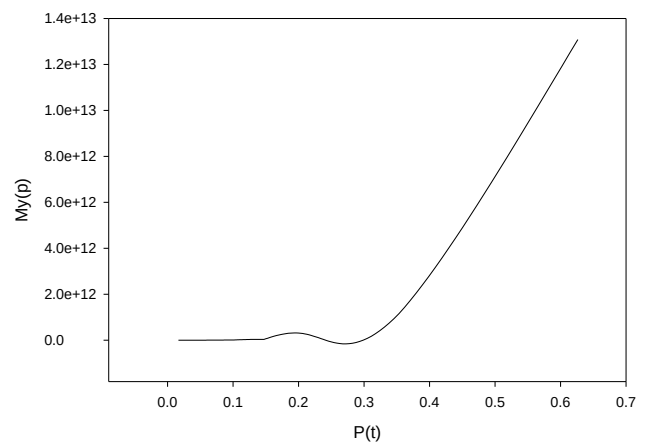
(h) 2D Graph of $My(p)$ and $P(t)$ for $n=3$, $A=2$



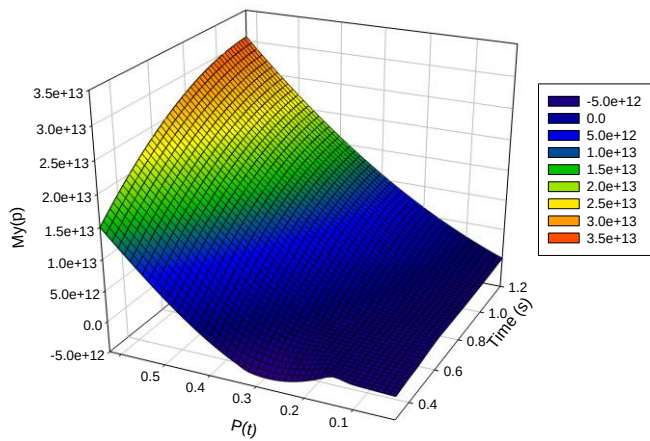
(i) 3D Graph of $My(p)$, $P(t)$ and $t(s)$ for $n=4$, $A=2$



(j) 2D Graph of $My(p)$ and $P(t)$ for $n=4$, $A=2$



(k) 3D Graph of $My(p)$, $P(t)$ and $t(s)$ for $n=5$, $A=2$



(l) 2D Graph of $My(p)$ and $P(t)$ for $n=5$, $A=2$

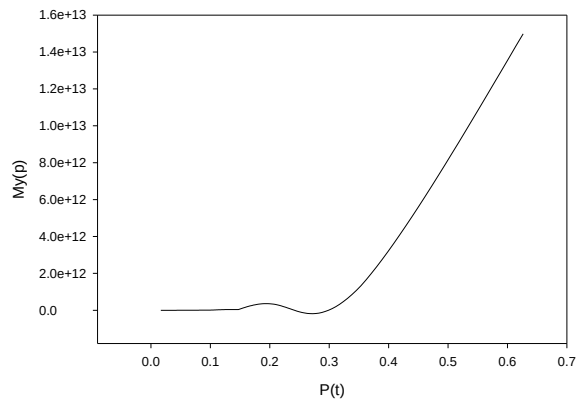
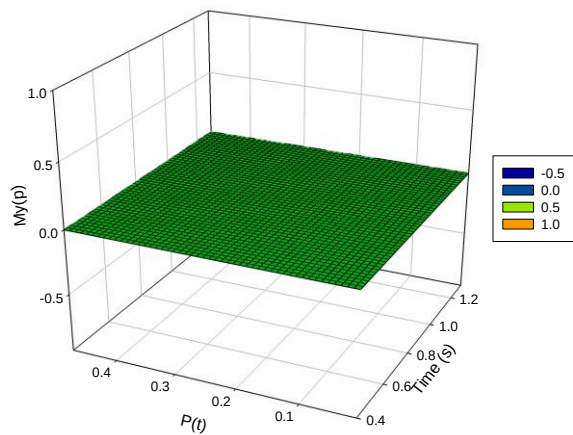
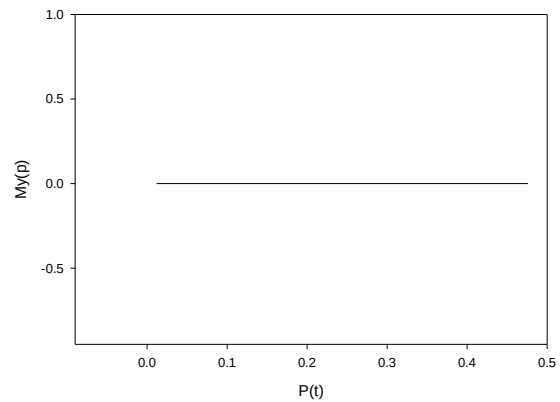


Fig 13. 1: 3 D & 2 D graph of equation (3.29d) for $A=2$, $Mo \neq 0$, (a) $n=0$ (b) $n=0$, (c) $n=1$, (d) $n=1$, (e) $n=2$, (f) $n=2$, (g) $n=3$, (h) $n=3$, (i) $n=4$, (j) $n=4$, (k) $n=5$, (l) $n=5$, for 3D and 2D respectively.

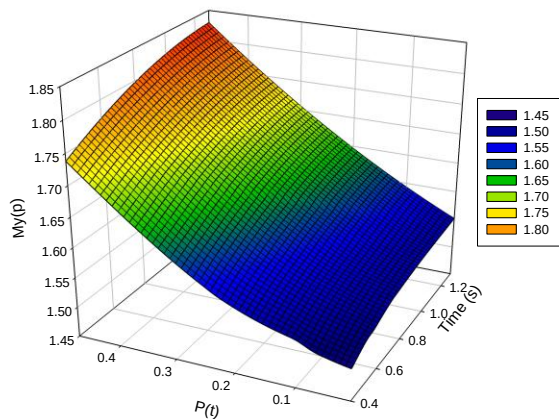
(a) 3D Graph of $My(p)$, $P(t)$ and $t(s)$ for $n=0$, $A=3$



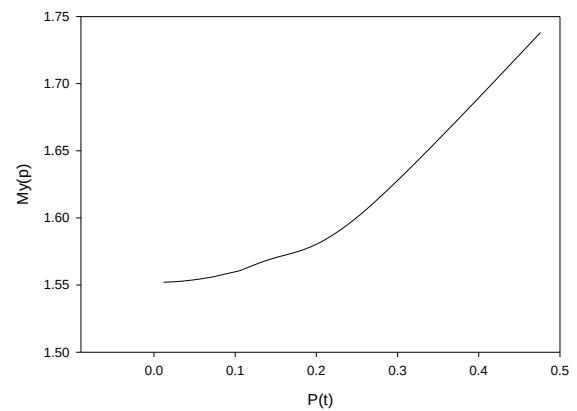
(b) 2D Graph of $My(p)$ and $P(t)$ for $n=0$, $A=3$



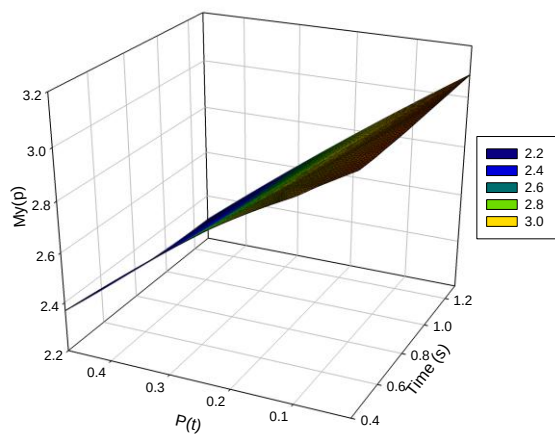
(c) 3D Graph of $My(p)$, $P(t)$ and $t(s)$ for $n=1$, $A=3$



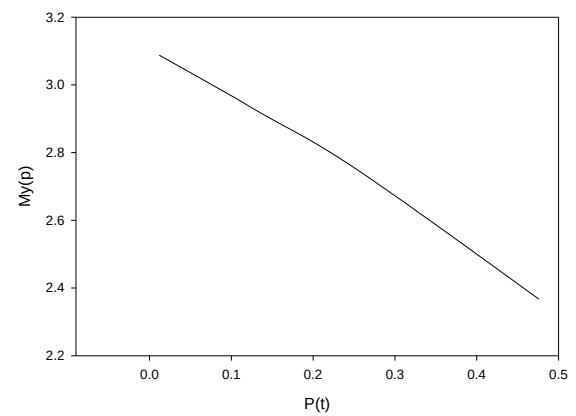
(d) 2D Graph of $My(p)$ and $P(t)$ for $n=1$, $A=3$



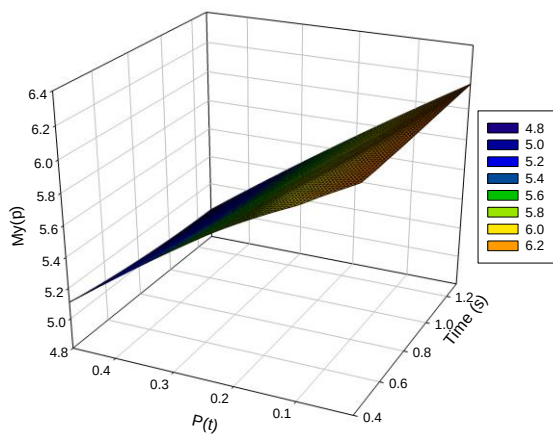
(e) 3D Graph of $My(p)$, $P(t)$ and $t(s)$ for $n=2$, $A=3$



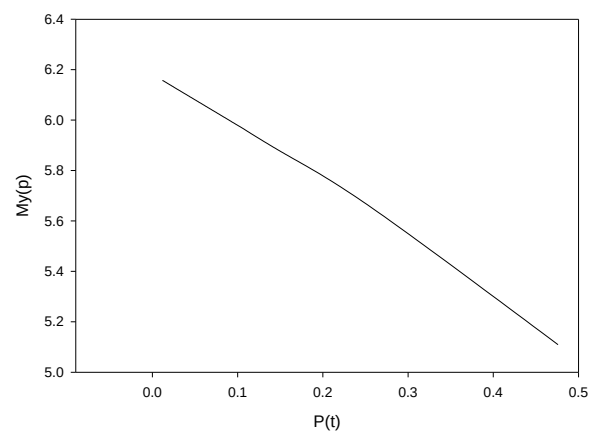
(f) 2D Graph of $My(p)$, $P(t)$ and $t(s)$ for $n=2$, $A=3$



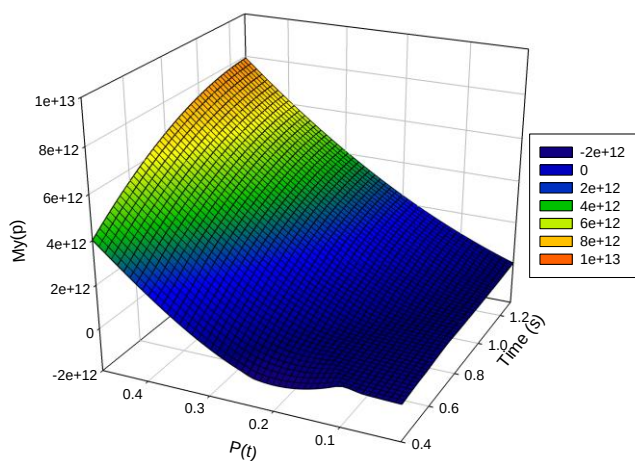
(g) 3D Graph of $My(p)$, $P(t)$ and $t(s)$ for $n=3$, $A=3$



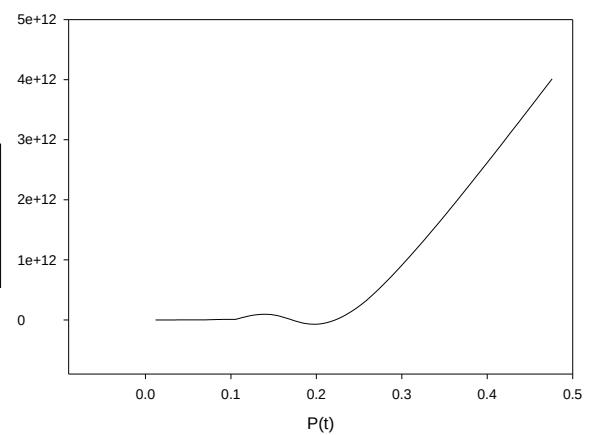
(h) 2D Graph of $My(p)$, $P(t)$ and $t(s)$ for $n=3$, $A=3$



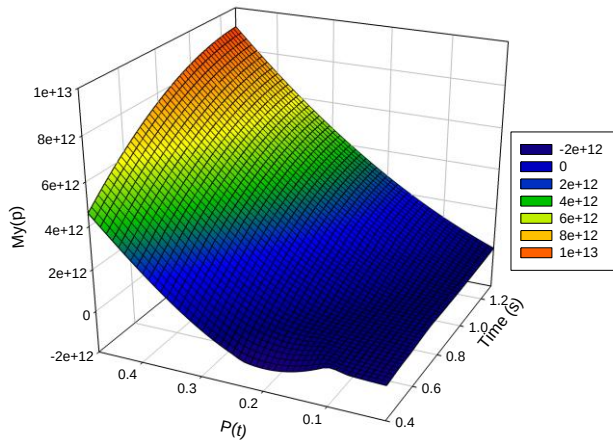
(i) 3D Graph of $My(p)$, $P(t)$ and $t(s)$ for $n=4$, $A=3$



(j) 2D Graph of $My(p)$ and $P(t)$ for $n=4$, $A=3$



(k) 3D Graph of $My(p)$, $P(t)$ and $t(s)$ for $n=5$, $A=3$



(l) 2D Graph of $My(p)$ and $P(t)$ for $n=5$, $A=3$

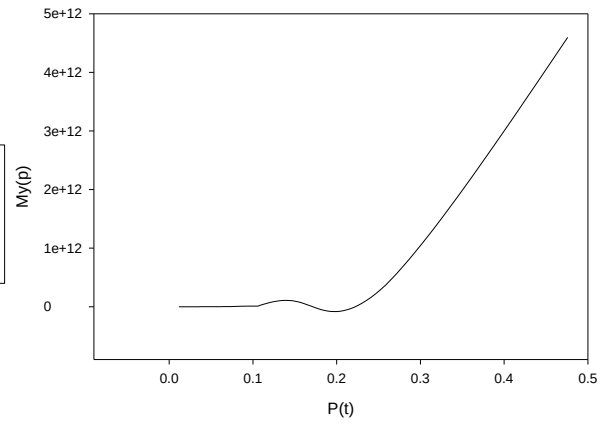
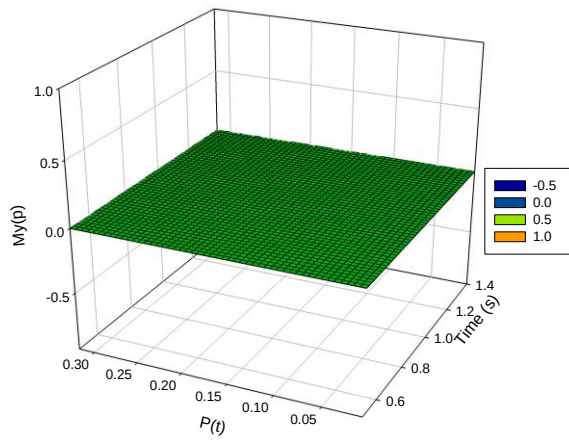
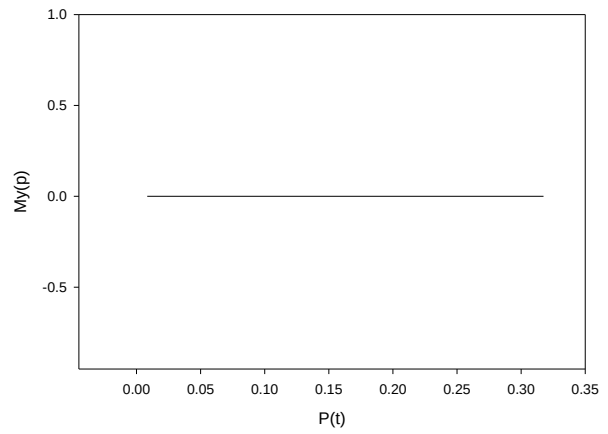


Fig 13.2: 3 D & 2 D graph of equation (3.29d) for $A=3$, $Mo \neq 0$, (a) $n=0$ (b) $n=0$, (c) $n=1$, (d) $n=1$, (e) $n=2$, (f) $n=2$, (g) $n=3$, (h) $n=3$, (i) $n=4$, (j) $n=4$, (k) $n=5$, (l) $n=5$, for 3D and 2D respectively.

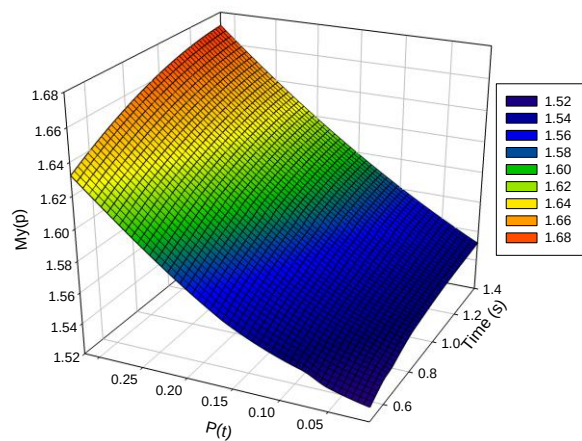
(a) 3D Graph of $My(p)$, $P(t)$ and $t(s)$ for $n=0$, $A=4$



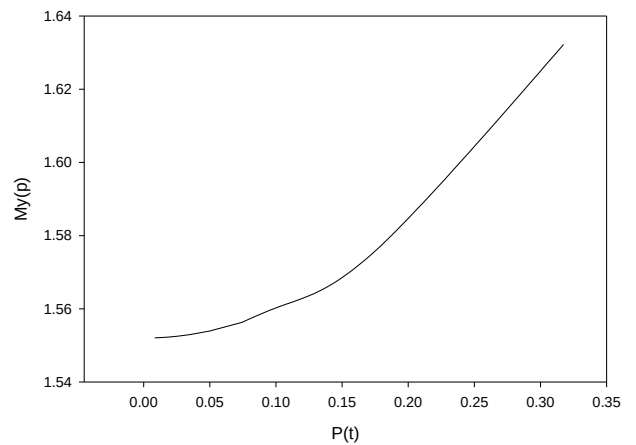
(b) 2D Graph of $My(p)$ and $P(t)$ for $n=0$, $A=4$



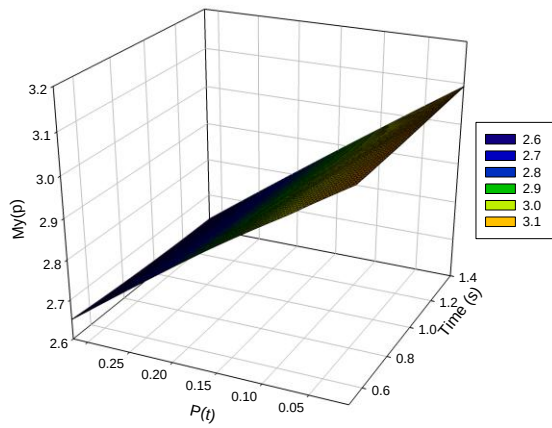
(c) 3D Graph of $My(p)$, $P(t)$ and $t(s)$ for $n=1$, $A=4$



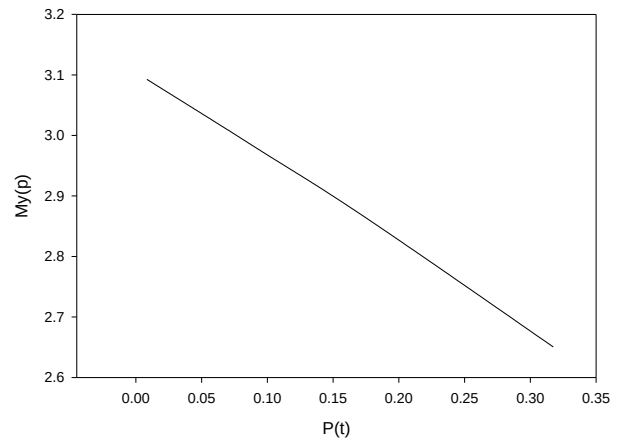
(d) 2D Graph of $My(p)$ and $P(t)$ for $n=1$, $A=4$



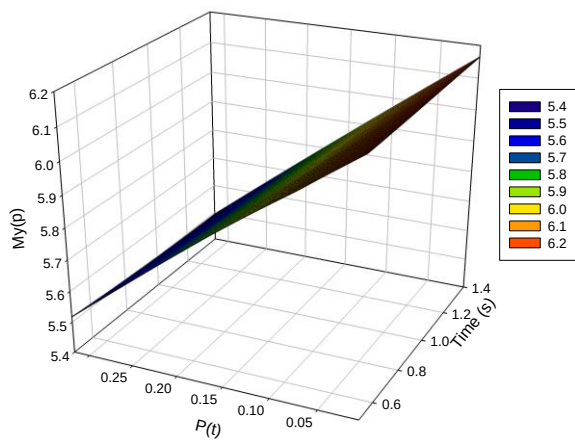
(e) 3D Graph of $My(p)$, $P(t)$ and $t(s)$ for $n=2$, $A=4$



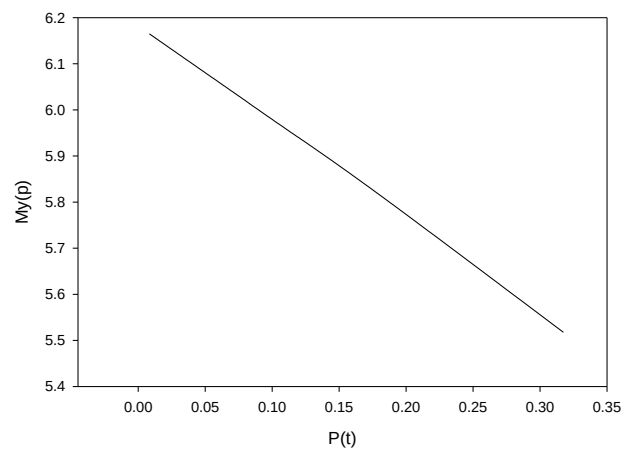
(f) 2D Graph of $My(p)$ and $P(t)$ for $n=2$, $A=4$



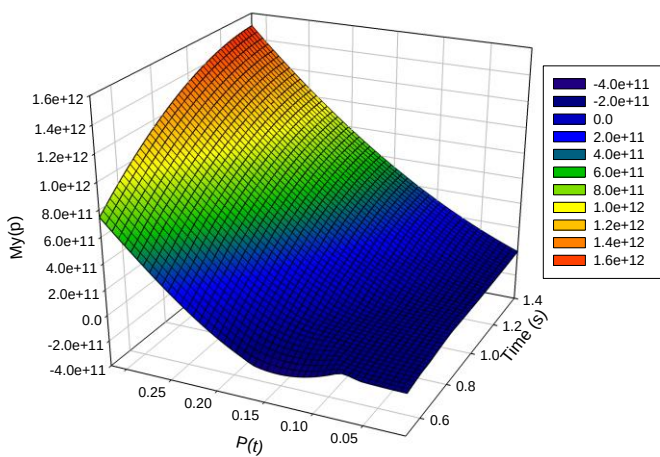
(g) 3D Graph of $My(p)$, $P(t)$ and $t(s)$ for $n=3$, $A=4$



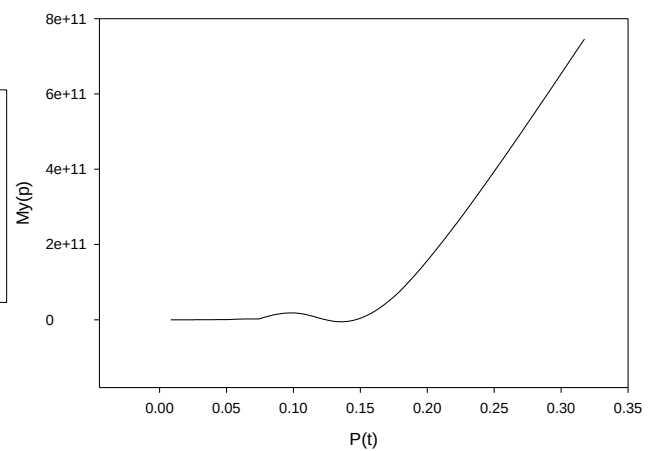
(h) 2D Graph of $My(p)$ and $P(t)$ for $n=3$, $A=4$



(i) 3D Graph of $My(p)$, $P(t)$ and $t(s)$ for $n=4$, $A=4$



(j) 2D Graph of $My(p)$ and $P(t)$ for $n=4$, $A=4$



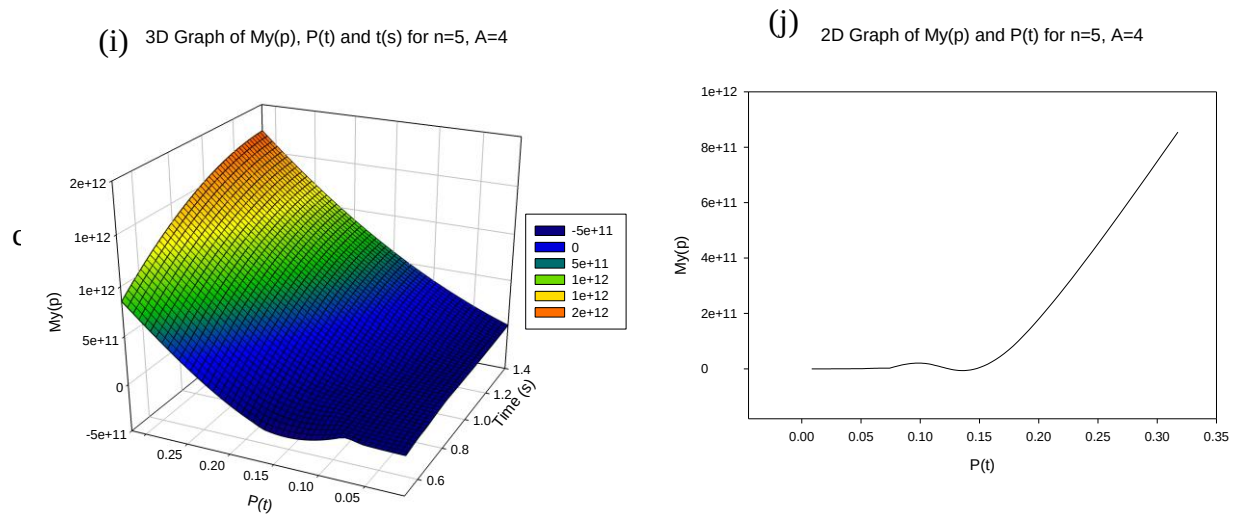
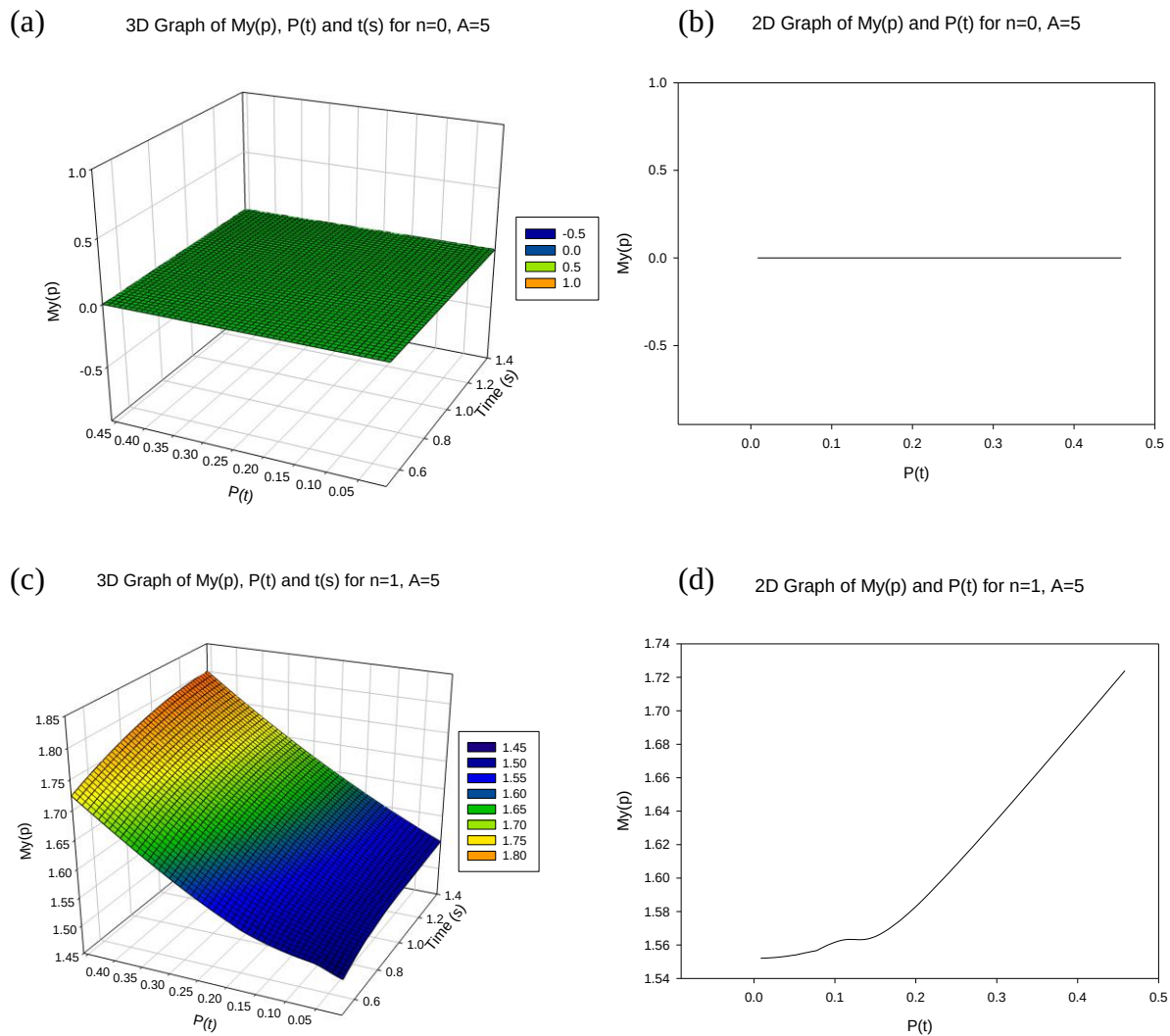
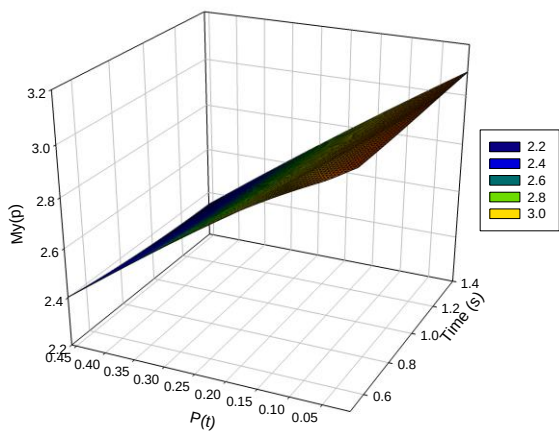


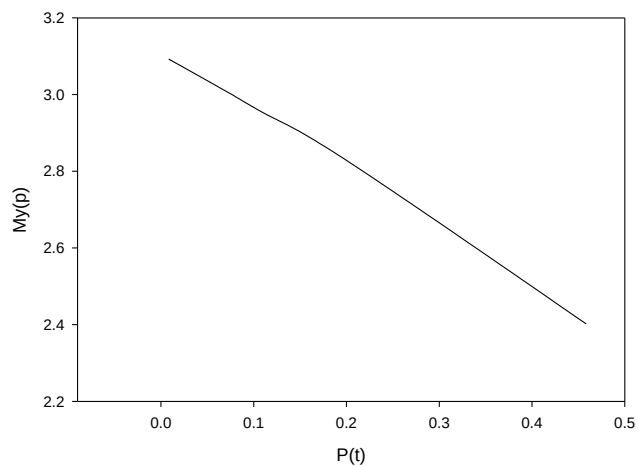
Fig 14: 3 D & 2 D graph of equation (3.29d) for $A=4$, $Mo \neq 0$, (a) $n=0$ (b) $n=0$, (c) $n=1$, (d) $n=1$, (e) $n=2$, (f) $n=2$, (g) $n=3$, (h) $n=3$, (i) $n=4$, (j) $n=4$, (k) $n=5$, (l) $n=5$, for 3D and 2D respectively.



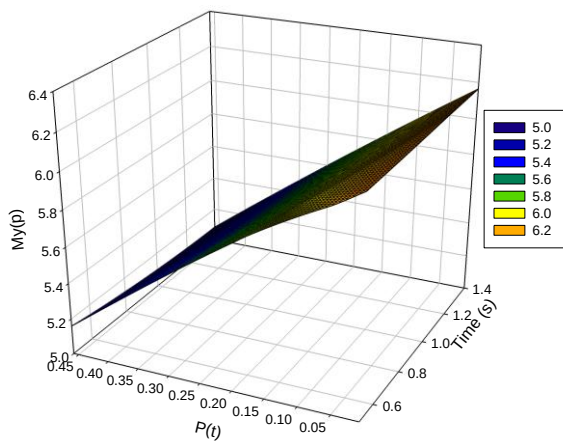
(e) 3D Graph of $My(p)$, $P(t)$ and $t(s)$ for $n=2$, $A=5$



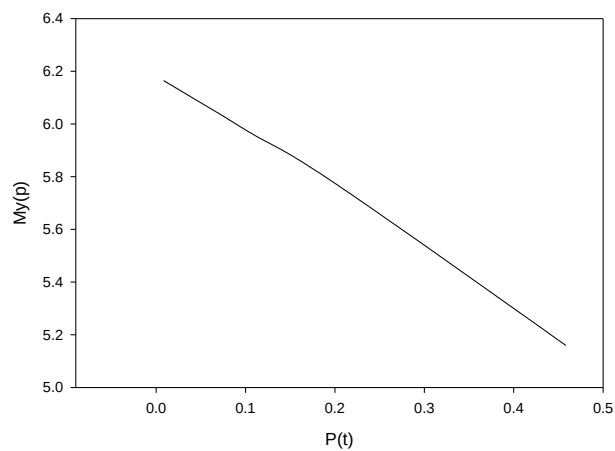
(f) 2D Graph of $My(p)$ and $P(t)$ for $n=2$, $A=5$



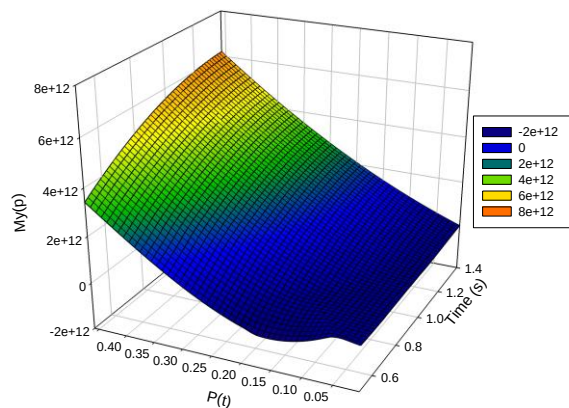
(g) 3D Graph of $My(p)$, $P(t)$ and $t(s)$ for $n=3$, $A=5$



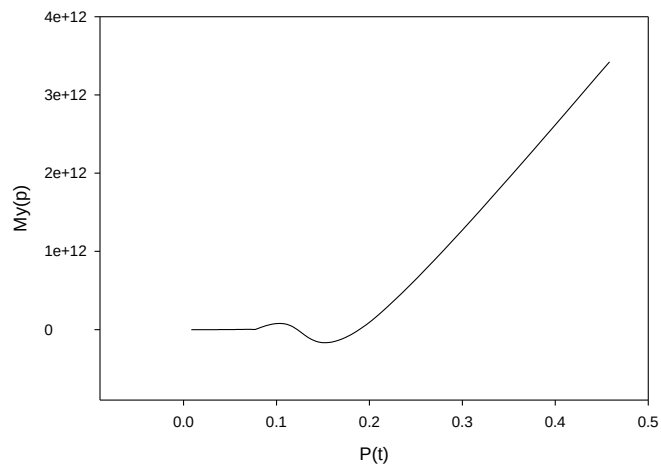
(h) 2D Graph of $My(p)$ and $P(t)$ for $n=3$, $A=5$



(i) 3D Graph of $My(p)$, $P(t)$ and $t(s)$ for $n=4$, $A=5$



(j) 2D Graph of $My(p)$ and $P(t)$ for $n=4$, $A=5$



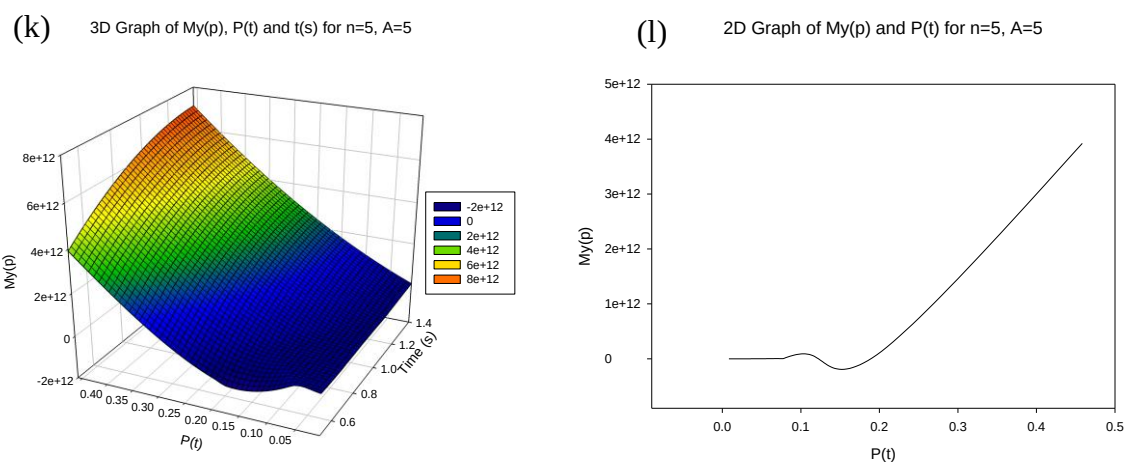


Fig 15: 3 D & 2 D graph of equation (3.29d) for $A=5$, $M_0 \neq 0$, (a) $n=0$ (b) $n=0$, (c) $n=1$, (d) $n=1$, (e) $n=2$, (f) $n=2$, (g) $n=3$, (h) $n=3$, (i) $n=4$, (j) $n=4$, (k) $n=5$, (l) $n=5$, for 3D and 2D respectively.

VARIATION OF $P(t)$ WITH TIME(S) FOR VARYING VALUES OF 'A' AND T_2

A condition in the solution of equation (1) gave rise to equation (4b). The solution for a case where 'A' = 0 defined the porosity. We solved equation (4b) for a physical case when A is not equal to zero and obtained a solution in equation (16) to show the influence of parameter A and spin-spin relaxation time (T_2) on porosity in porous media as shown in figures 18-22. The choice of T_2 relaxation time of 0.01 to 0.5 is typical of spin-spin relaxation time for blood flow.

It was observed that porosity become more exponential for T_2 relaxation time = 0.091 sec, while the constant A is varied from 1 to 5. A less significant full wave oscillation was also observed between time $t=0.3$ sec and 0.5 sec, as porosity increases, the time t for which porosity become measurable increases from 0.1 to 0.2 sec. This is a consequence of porosity becoming discontinuous at $t=0$ and 0.1 sec. Porosity again become more and more exponential for T_2 relaxation time = 0.172 sec while the constant A is varied from 1 to 5. A less and less significant oscillation was observed between time $t=0.3$ sec and 0.5 sec.

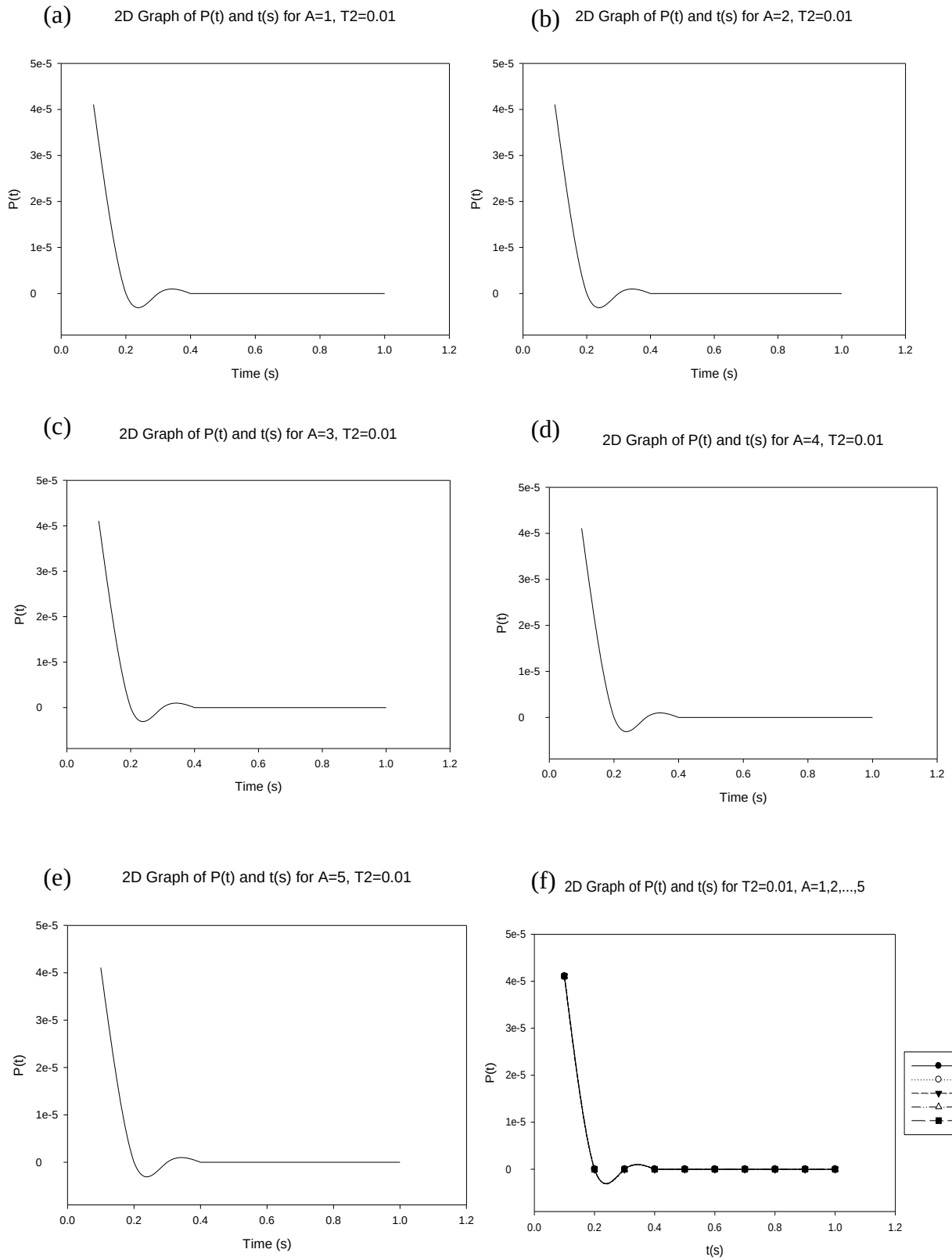
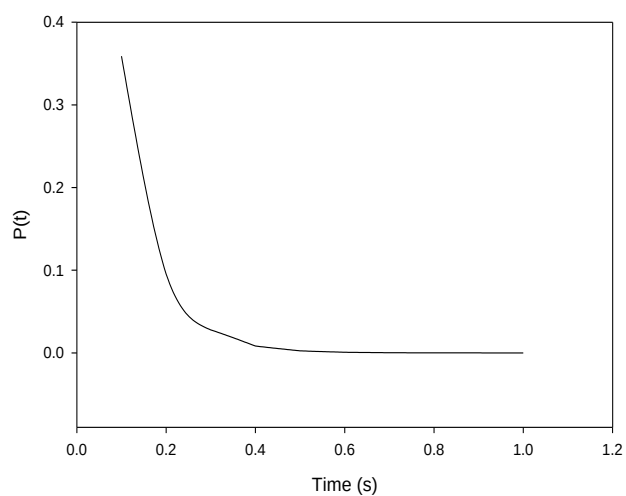
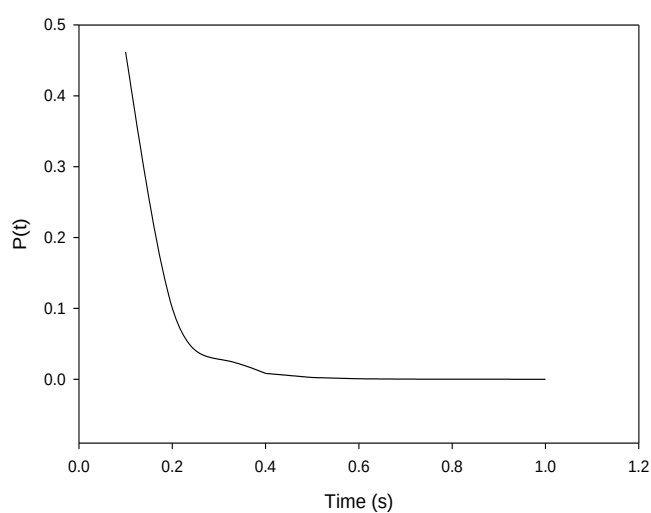


Fig 16: 2 D graph of equation (3.53) for $Mo \neq 0$, $T_2=0.01s$, (a) $A=1$, (b) $A=2$, (c) $A=3$, (d) $A=4$, (e) $A=5$ (f) $A=1,2,3,4,5$.

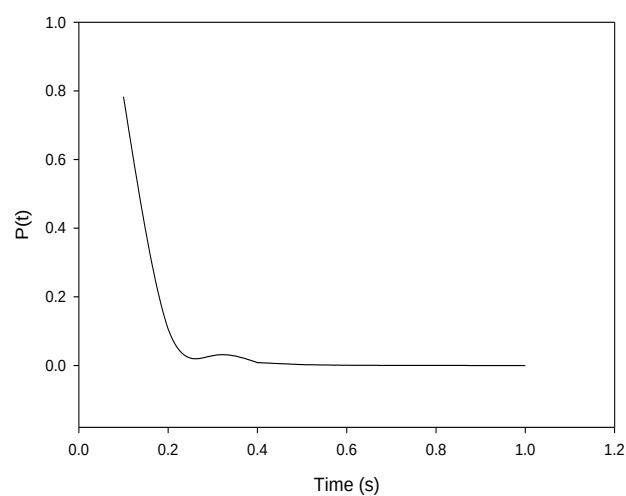
(a) 2D Graph of $P(t)$ and $t(s)$ for $A=1$, $T_2=0.091$



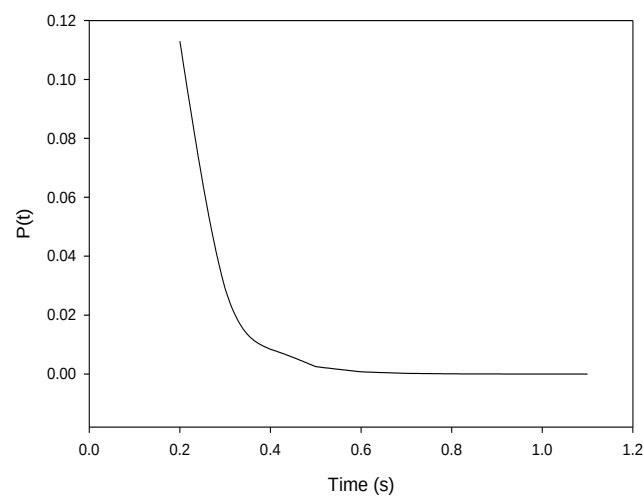
(b) 2D Graph of $P(t)$ and $t(s)$ for $A=2$, $T_2=0.091$



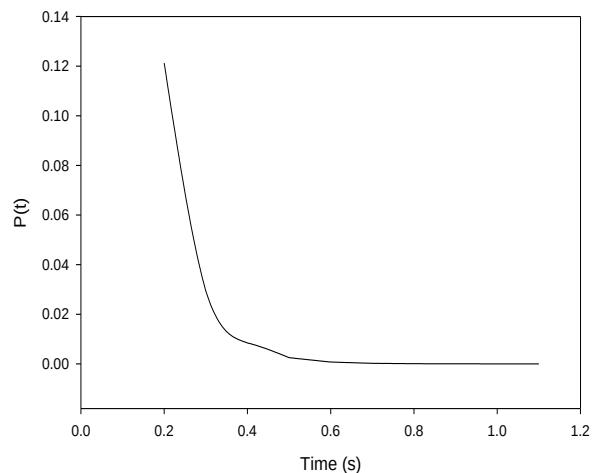
(c) 2D Graph of $P(t)$ and $t(s)$ for $A=3$, $T_2=0.091$



(d) 2D Graph of $P(t)$ and $t(s)$ for $A=4$, $T_2=0.091$



(e) 2D Graph of $P(t)$ and $t(s)$ for $A=5$, $T_2=0.091$



(f) 2D Graph of $P(t)$ and $t(s)$ for $T_2=0.091$ for $A=1, \dots, 5$

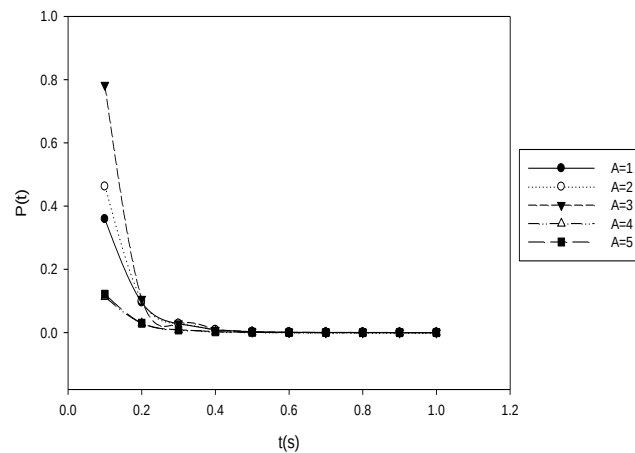
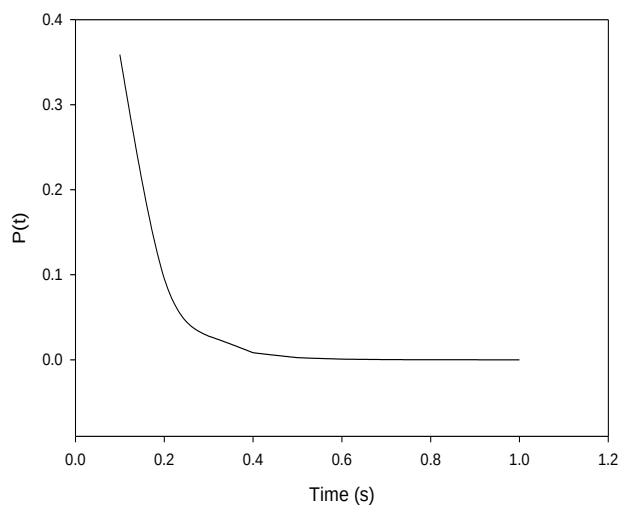
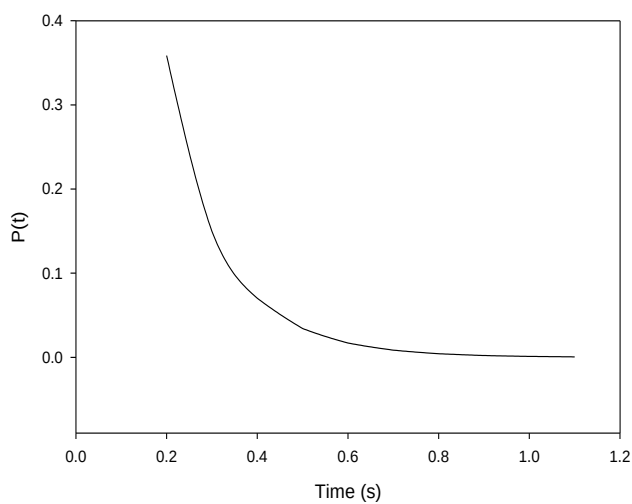


Fig 17: 2 D graph of equation (3.53) for $Mo \neq 0$, $T_2=0.091$ s, (a) $A=1$, (b) $A=2$, (c) $A=3$, (d) $A=4$, (e) $A=5$ (f) $A=1, 2, 3, 4, 5$.

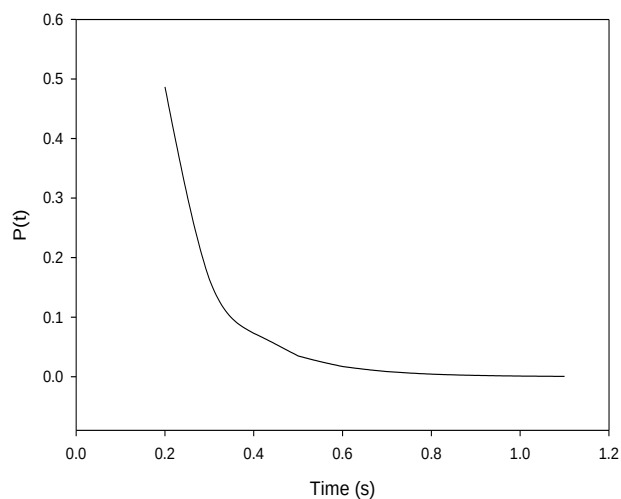
(a) 2D Graph of $P(t)$ and $t(s)$ for $A=1$, $T_2=0.172$



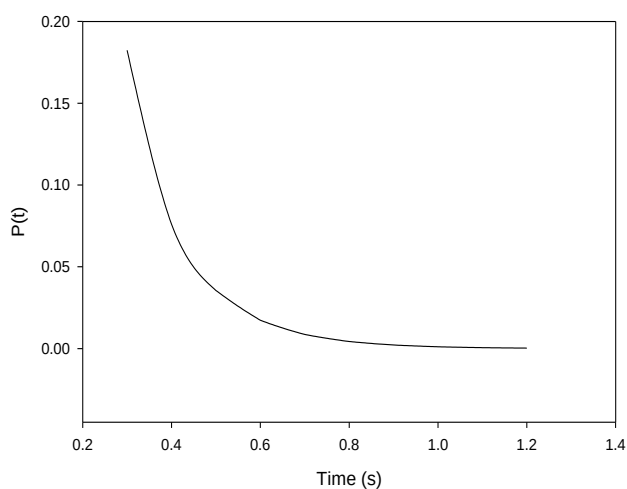
(b) 2D Graph of $P(t)$ and $t(s)$ for $A=2$, $T_2=0.172$



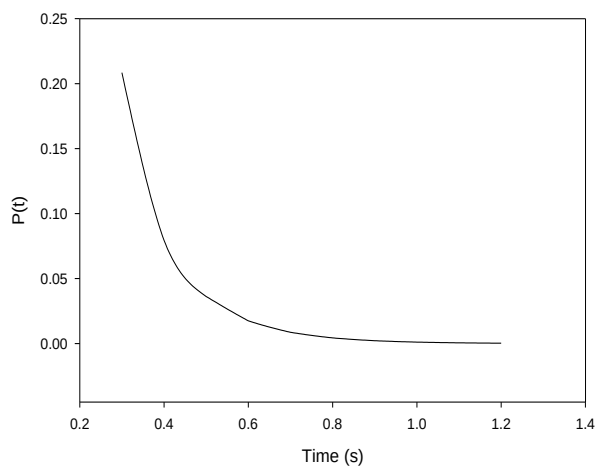
(c) 2D Graph of $P(t)$ and $t(s)$ for $A=3$, $T_2=0.172$



(d) 2D Graph of $P(t)$ and $t(s)$ for $A=4$, $T_2=0.172$



(e) 2D Graph of $P(t)$ and $t(s)$ for $A=5$, $T_2=0.172$



(f) 2D Graph of $P(t)$ and $t(s)$ for $T_2=0.172$, $A=1, \dots, 5$

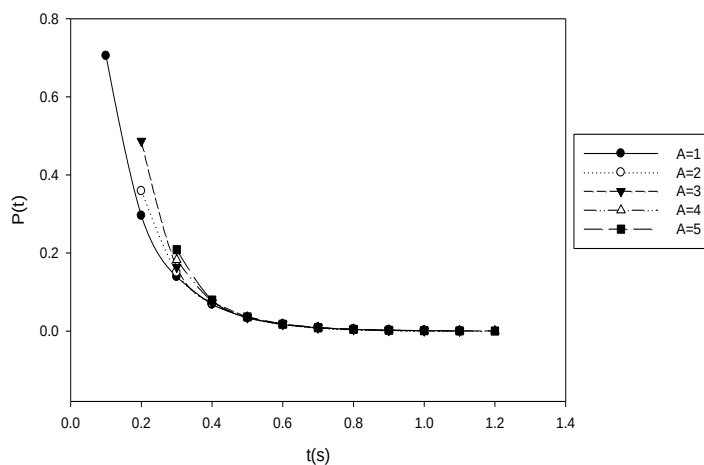
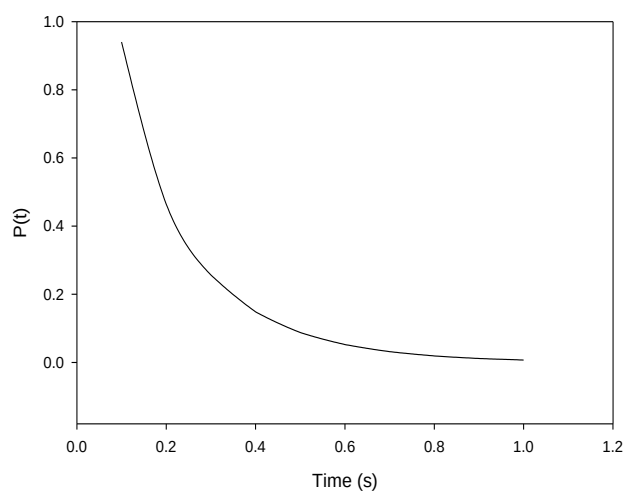
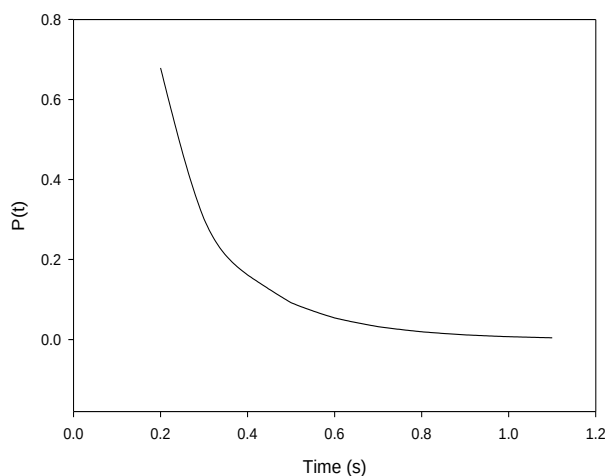


Fig 18: 2 D graph of equation (3.53) for $Mo \neq 0$, $T_2=0.172s$, (a) $A=1$, (b) $A=2$, (c) $A=3$, (d) $A=4$, (e) $A=5$ (f) $A=1, 2, 3, 4, 5$.

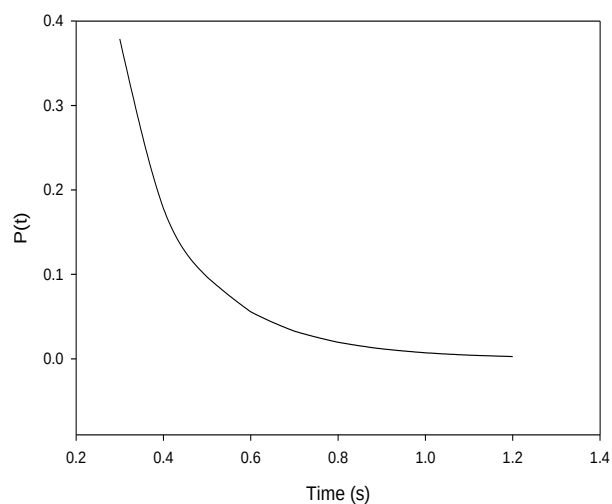
(a) 2D Graph of $P(t)$ and $t(s)$ for $A=1, T_2=0.253$



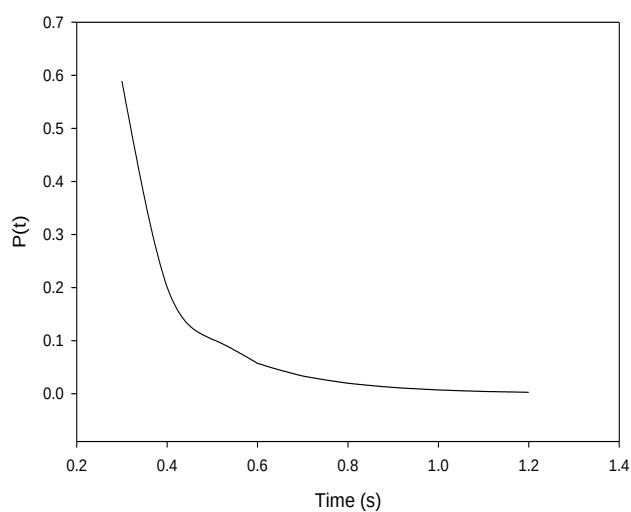
(b) 2D Graph of $P(t)$ and $t(s)$ for $A=2, T_2=0.253$



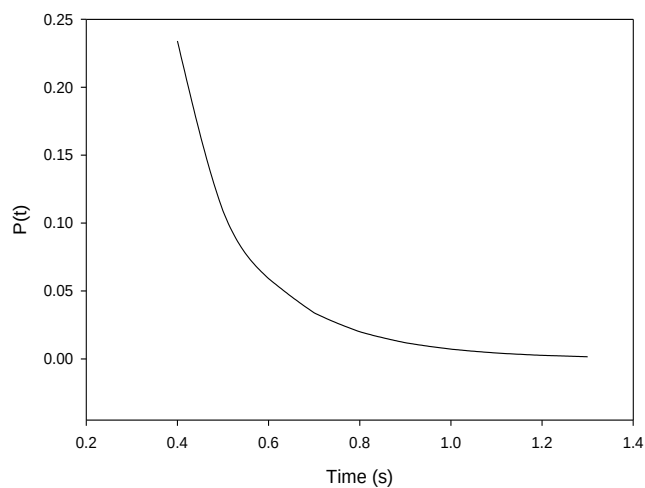
(c) 2D Graph of $P(t)$ and $t(s)$ for $A=3, T_2=0.253$



(d) 2D Graph of $P(t)$ and $t(s)$ for $A=4, T_2=0.253$



(e) 2D Graph of $P(t)$ and $t(s)$ for $A=5, T_2=0.253$



(f) 2D Graph of $P(t)$ and $t(s)$ for $T_2=0.253, A=1, \dots, 5$

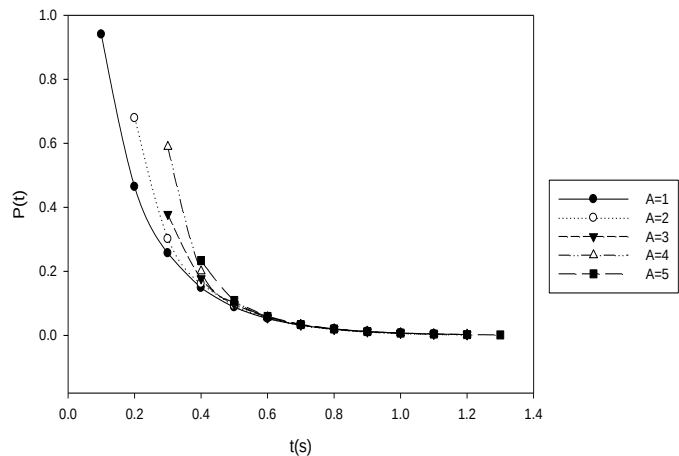
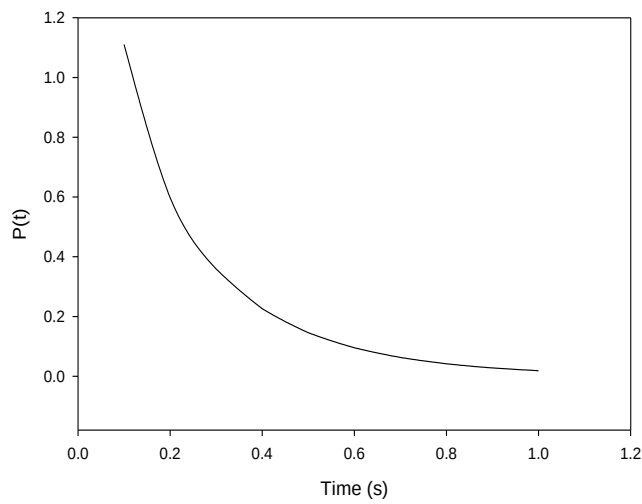
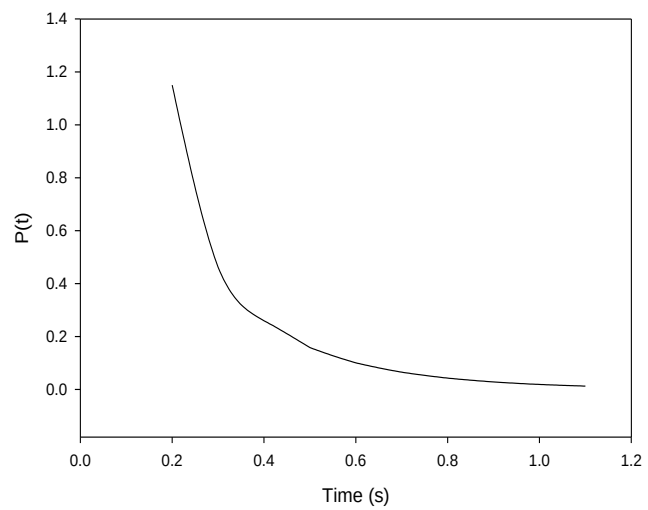


Fig 19: 2 D graph of equation (3.53) for $Mo \neq 0$, $T_2=0.253s$, (a) $A=1$, (b) $A=2$, (c) $A=3$, (d) $A=4$, (e) $A=5$ (f) $A=1, 2, 3, 4, 5$.

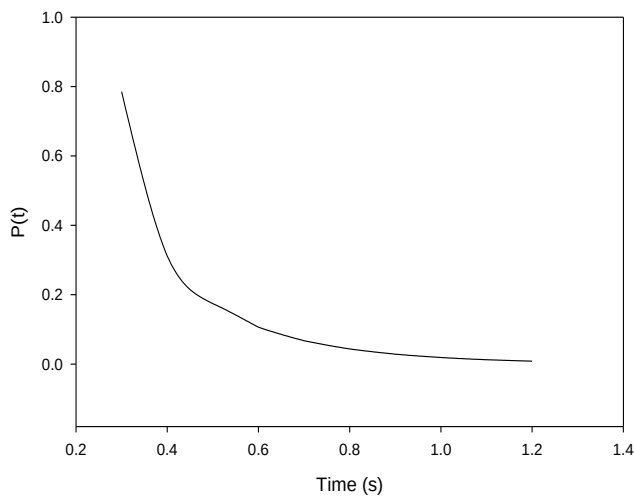
(a) 2D Graph of $P(t)$ and $t(s)$ for $A=1$, $T_2=0.334$



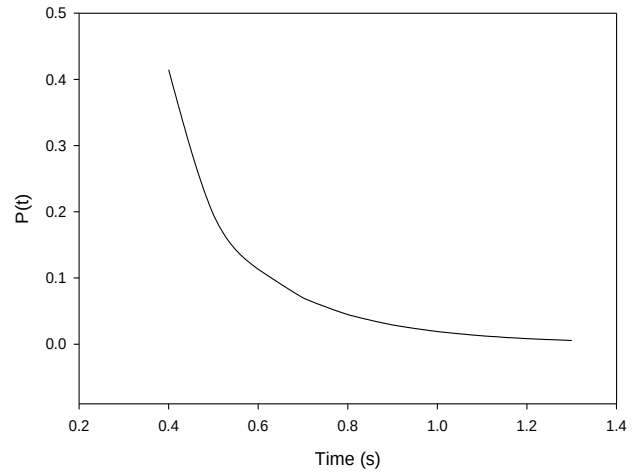
(b) 2D Graph of $P(t)$ and $t(s)$ for $A=2$, $T_2=0.334$



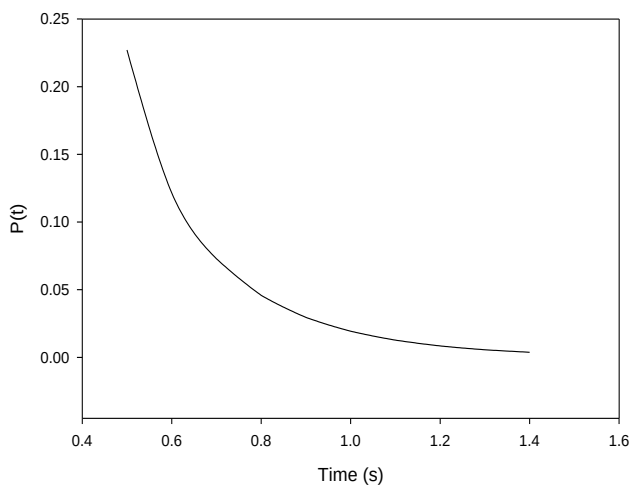
(c) 2D Graph of $P(t)$ and $t(s)$ for $A=3$, $T_2=0.334$



(d) 2D Graph of $P(t)$ and $t(s)$ for $A=4$, $T_2=0.334$



(e) 2D Graph of $P(t)$ and $t(s)$ for $A=5$, $T_2=0.334$



(f) 2D Graph of $P(t)$ and $t(s)$ for $T_2=0.334, A=1, \dots, 5$

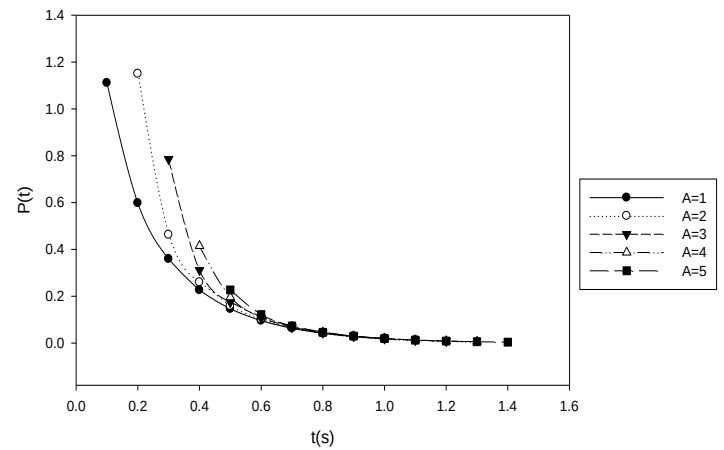
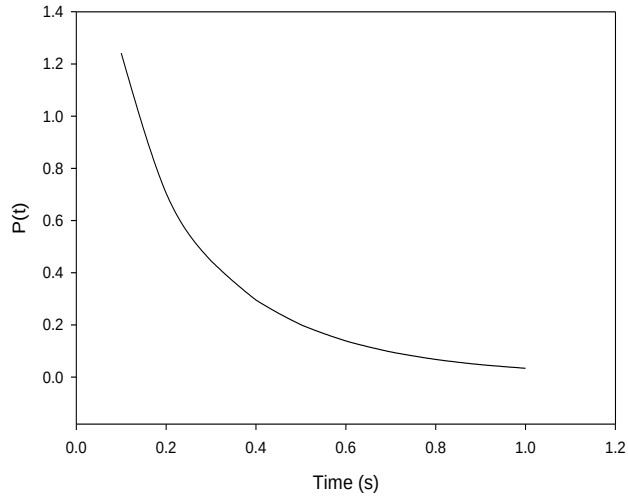
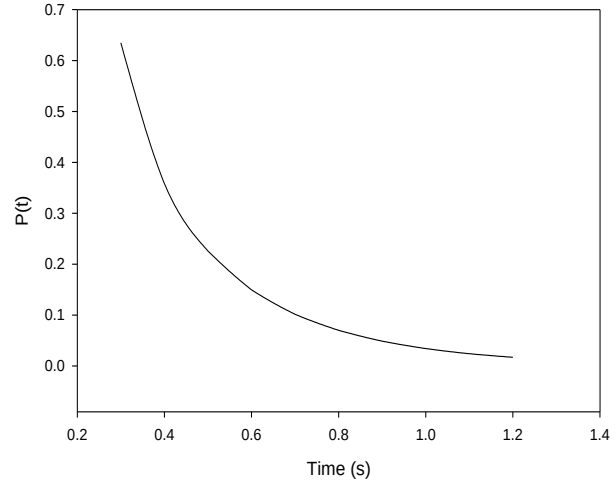


Fig 20: 2 D graph of equation (3.53) for $Mo \neq 0$, $T_2=0.334s$, (a) $A=1$, (b) $A=2$, (c) $A=3$, (d) $A=4$, (e) $A=5$ (f) $A=1, 2, 3, 4, 5$.

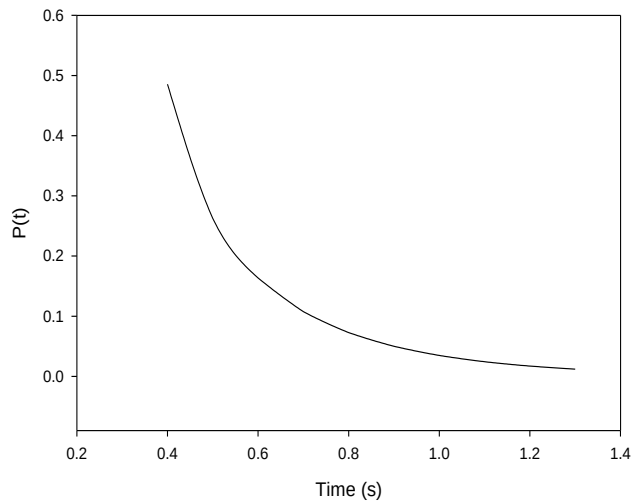
(a) 2D Graph of $P(t)$ and $t(s)$ for $A=1$, $T_2=0.415$



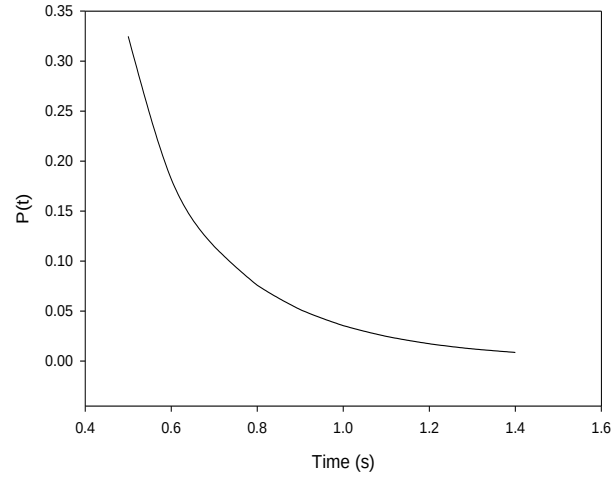
(b) 2D Graph of $P(t)$ and $t(s)$ for $A=2$, $T_2=0.415$



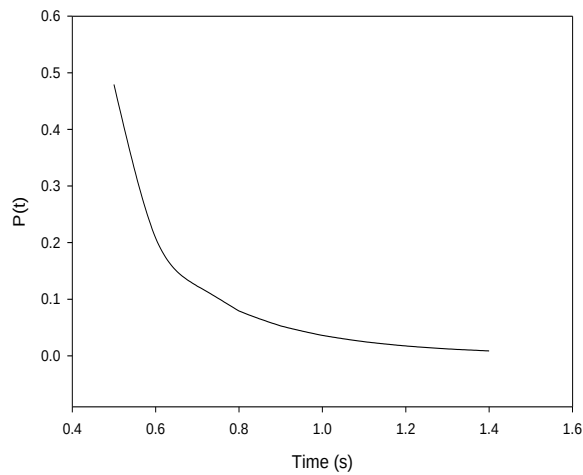
(c) 2D Graph of $P(t)$ and $t(s)$ for $A=3$, $T_2=0.415$



(d) 2D Graph of $P(t)$ and $t(s)$ for $A=4$, $T_2=0.415$



(e) 2D Graph of $P(t)$ and $t(s)$ for $A=5$, $T_2=0.415$



(f) 2D Graph of $P(t)$ and $t(s)$ for $T_2=0.415$, $A=1, \dots, 5$

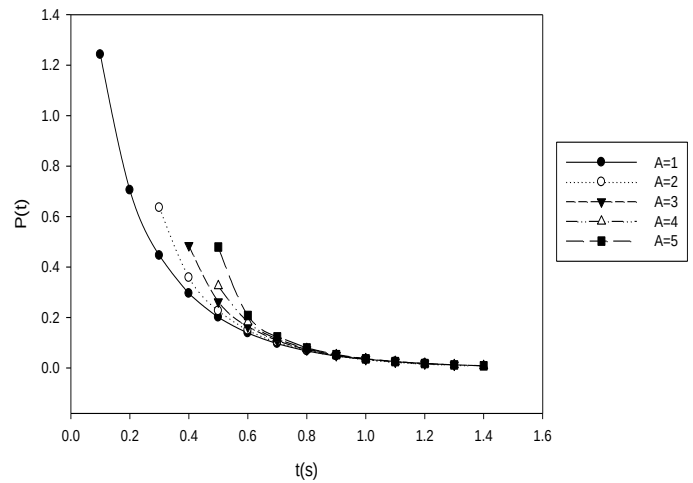
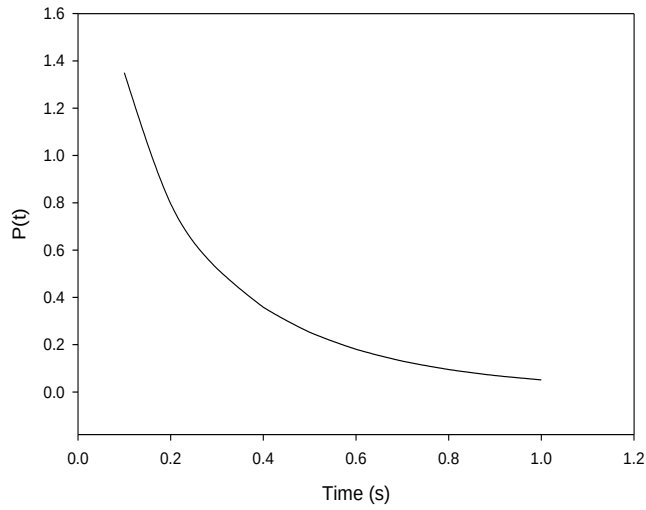
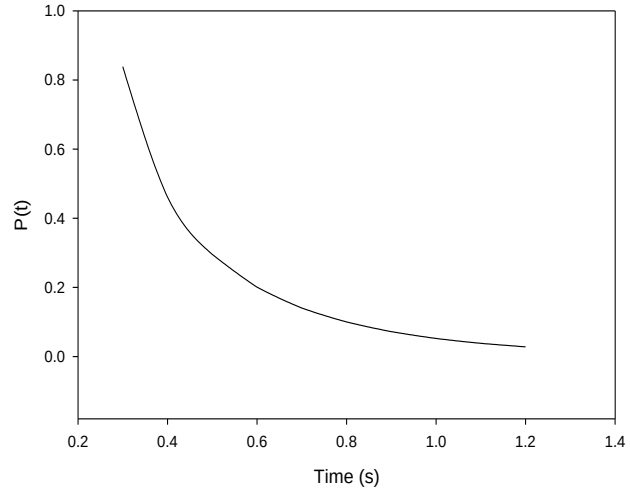


Fig 21: 2 D graph of equation (3.53) for $Mo \neq 0$, $T_2=0.415s$, (a) $A=1$, (b) $A=2$, (c) $A=3$, (d) $A=4$, (e) $A=5$ (f) $A=1, 2, 3, 4, 5$.

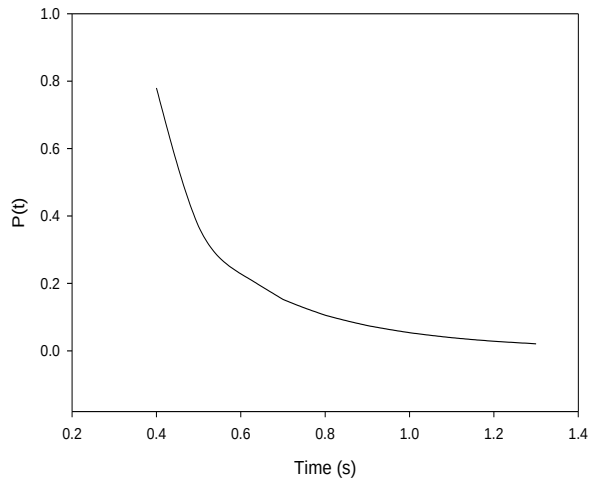
(a) 2D Graph of $P(t)$ and $t(s)$ for $A=1$, $T_2=0.500$



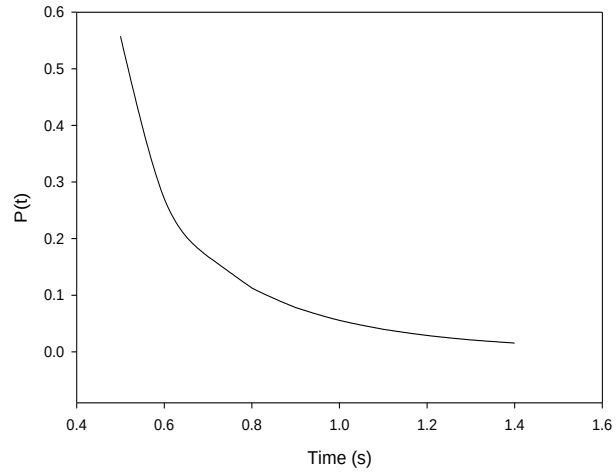
(b) 2D Graph of $P(t)$ and $t(s)$ for $A=2$, $T_2=0.50$



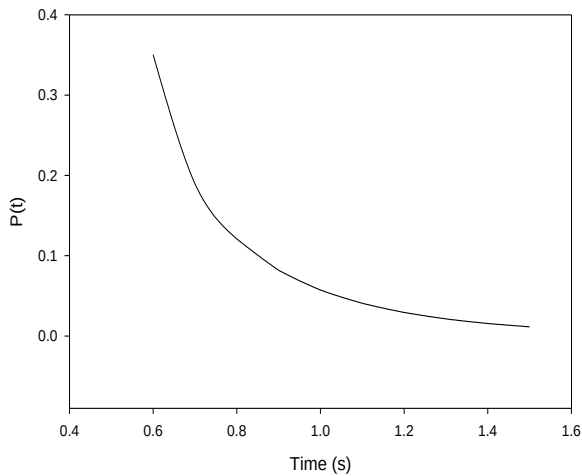
(c) 2D Graph of $P(t)$ and $t(s)$ for $A=3$, $T_2=0.500$



(d) 2D Graph of $P(t)$ and $t(s)$ for $A=4$, $T_2=0.500$



(e) 2D Graph of $P(t)$ and $t(s)$ for $A=5$, $T_2=0.500$



(f) 2D Graph of $P(t)$ and $t(s)$ for $T_2=0.5, A=1, \dots, 5$

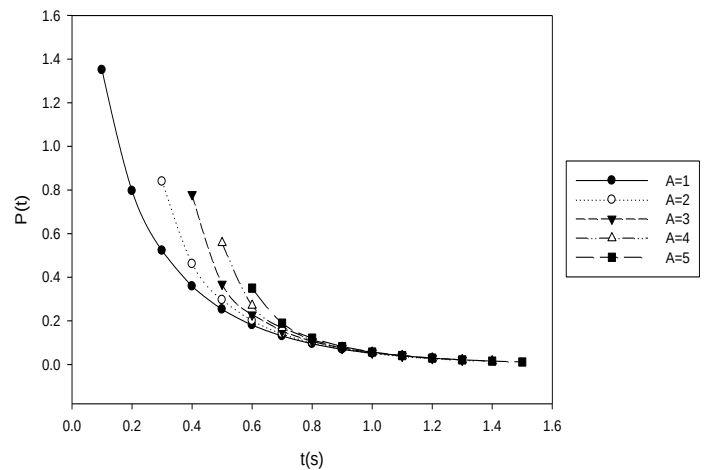


Fig 22: 2 D graph of equation (3.53) for $Mo \neq 0$, $T_2=0.50s$, (a) $A=1$, (b) $A=2$, (c) $A=3$, (d) $A=4$, (e) $A=5$ (f) $A=1, 2, 3, 4, 5$.

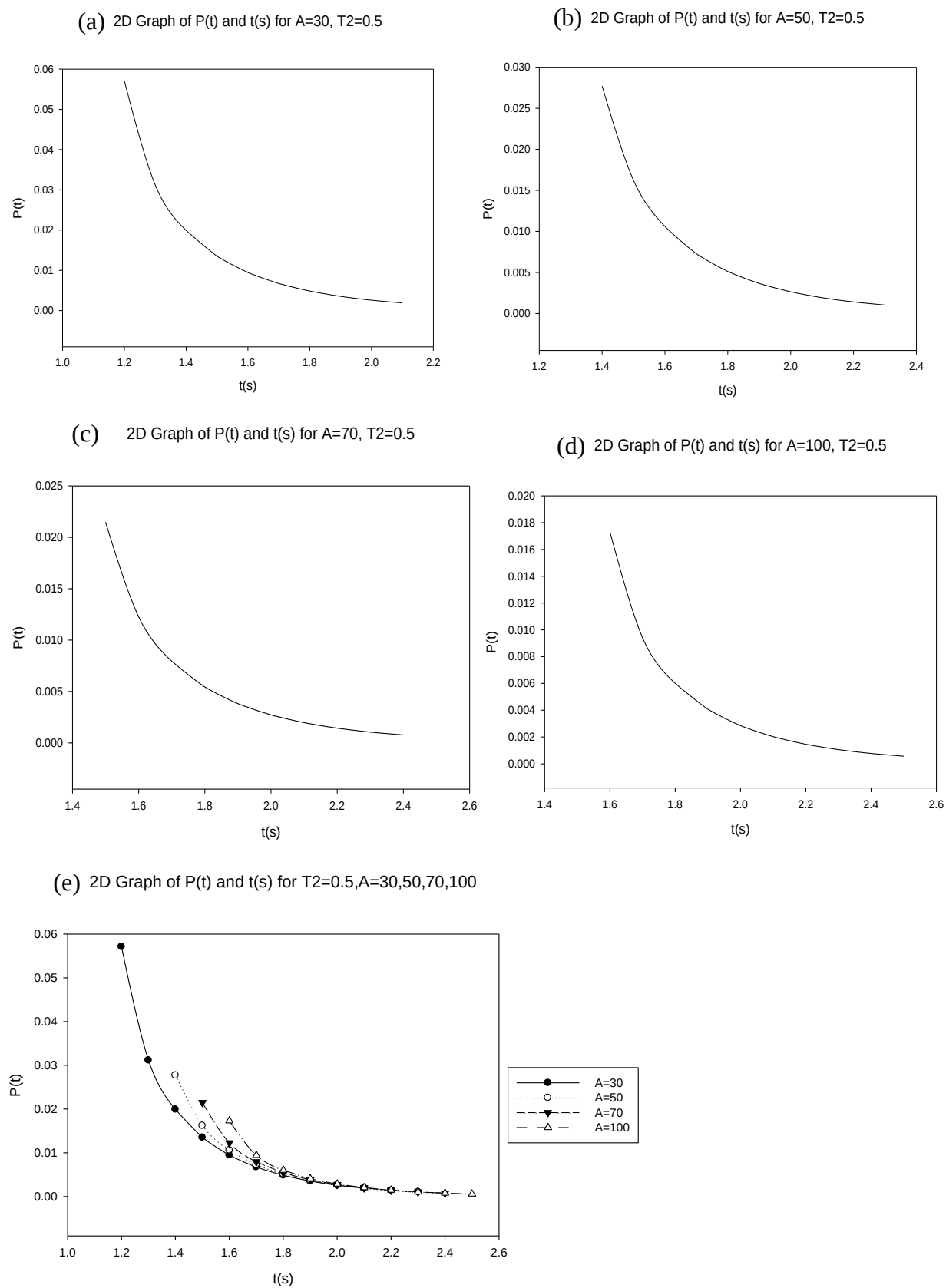


Fig 23: 2 D graph of equation (3.53) for $Mo \neq 0$, $T_2=0.50s$, (a) $A=30$, (b) $A=50$, (c) $A=70$, (d) $A=100$, (e) $A=30, 50, 70, 100$.

CONCLUSION

We have presented analytical solution to time dependent Bloch equation for computational analysis of nano particles in porous media. Since the nano particle is expected to be imaged in a nano-porous medium (blood flow), we apply the transformation which make the transverse magnetization in time domain $M_y(t)$ measurable in the porous medium as $M_y(p)$ based on the condition that a^2 in equation (4) must be a positive integer and 'A' must be a constant. These conditions transforms $M_y(t)$ in a porous medium with porosity $p(t)$. The computational analyses of our results as presented in figures (1-23) that show influence of parameter A on both the NMR transverse magnetization and the porosity P (t). A simple solution of equation (6) when

$$a^2 = \frac{8\pi^2 mE}{h^2} \quad (18)$$

is given as

$$M_y(p) = N \sin ap \quad (19)$$

Equation (6) therefore becomes the Schrödinger's equation describing a nano particle moving in a porous medium with porosity p without any external force acting on it. The transverse magnetization in equation (19) is finite, single valued and continuous for all values of a and p . If the value of p vary from 0 to a maximum β , the porosity p and $p + \beta$ may represent the same point. The property of single valued NMR transverse magnetization denotes that,

$$M_y(p) = M_y(p + \beta) \quad (20)$$

and

$$\sin ap = \sin a(p + \beta) \quad (21)$$

Equation (21) is possible only if

$$a = 0, \pm 1, \pm 2, \pm 3, \pm 4, \pm 5, \dots \quad (22)$$

Based on equations (18, 22), it is observed that equation (10) describes nano particle as a simple harmonic oscillator with Hermite polynomials as the NMR transverse magnetization in porous media. From equation (18), the energy of a nano particle of mass m in a porous medium is

$$E = \frac{a^2 h^2}{8\pi^2 m} \quad (23)$$

Equation (9) can be useful to determine porosity based on the fast diffusion limit, the dominant term in T_2 and T_1 surface relaxation times in porous media is given by:

$$\frac{1}{T_{2surface}} = \rho_2 \left(\frac{S}{V} \right)_{pore} \quad (24)$$

$$\frac{1}{T_{1surface}} = \rho_1 \left(\frac{S}{V} \right)_{pore}$$

where

$\rho_2 = T_2$ surface relaxivity (T_2 relaxing strength of the grain surface)

$\rho_1 = T_1$ surface relaxivity (T_1 relaxing strength of the grain surface)

$\left(\frac{S}{V}\right)_{pore}$ = ratio of pore surface to fluid volume. The porosity in each of the pores in the porous

media based on equation (9) can be calculated as

$$p = p(t) = p_0 \left[e^{-\rho_1 \left(\frac{S}{V}\right)_{pore} t} + e^{-\rho_2 \left(\frac{S}{V}\right)_{pore} t} \right] \quad (25)$$

For example when all pores are assumed to have similar geometric shape, the largest pores have the lowest S/V and thus the longest T_2 . Medium-size pores have smaller S/V, yielding shorter T_2 values. The smallest pores have the highest S/V and the shortest T_2 values. For a single pore, the porosity $P(t)$ decays exponentially, and the porosity p_0 is proportional to the volume of fluid in the pore. When the complete distribution of the 100% water-saturated pores is considered the pores exhibit a distribution of T_2 [12]. The detailed application of this fundamental solution to explain and solve real life flow problems in which NMR -sensitive materials are transported through a small sized pore will be presented separately.

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