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Numerical Computation of NMR Magnetization for Various Tissues in the Human Body Using Oringinpro

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Abstract: Nuc1ear magnetic resonance (NMR) spectroscopy and imaging are arguab1y the most versati1e techniques use in biomedica1 research today. NMR spectroscopy is a powerfu1 and theoretica1 ana1ytica1 too1s. Since the deve1opment of NMR spectroscopy it is has become a very important too1s in the fie1d of medicine because of it being safer than the X-ray crysta11ography which has radiation effects on the human body. The most attractive features of NMR techniques are the wide range of bio1ogica1 processes that can be investigated using these methods and the variety and versati1ity of the specific MR techniques that can be app1ied. diagnosis of diseases. With the advent of computer programme, different computer programme has a1so being deve1oped for NMR spectroscopy for performing different ana1ysis on how e1ectromagnetic radiation interact with various form of matter. This research perform NMR ana1ysis of different tissue in the human body using Originpro. The research investigates various tissues of the human body, with the aid of Bloch flow equation the research obtained the transverse magnetization equation that was used for the tranverse magnetization map for the different tissues. Three different relaxation times consider for the different biological tissues are 0.5 T, 1.0 T and 1.5 T. The transverse magnetization for the various tissues are ca1cu1ated at different magnetic f1ux density, at range of 0-0.02 seconds and a length for the tissues were in the range of $4.5x10^{-12}$ to $4.5x10^{-}$m. The result shows that transverse magnetization was greater at 0.5 T for the tissues considered at the range of $4.5x10^{-12}$ to $4.5x10^{-5}$ m.

Keywords: Bloch Equation, NMR, Relaxation time, Tissues, OriginPro

Introduction

Nuclear magnetic resonance which is commonly abbreviated as NMR by scientists is a physical phenomenon when the nucleus of certain atoms is immersed in a static magnetic field and exposed to another oscillating magnetic field. NMR also refers to a physical principle response of nuclei to a magnetic field (Grover et al., 2015). Many nuclei possess magnetic moment, they act like spinning bar magnets. These spinning bar magnetic nuclei interact with externally applied magnetic fields, producing measurable signals (Levitt, 2013).

The phenomenon of NMR has been known since 1946 and is widely used as an analytical tool in physics and chemistry (Reid et al., 1982). At approximately the same time, it was demonstrated that the use of magnetic field gradients could be used to encode NMR signals spatially (Cooley et al., 2015), and thus the concept of magnetic resonance imaging (MRI) was born. Soon thereafter, MR images of the human body were obtained and as early as l980, the evaluation of MRI as a clinically useful imaging modality had started (Mammarappallil et al., 2019).

Spectroscopy is the study of how electromagnetic radiation such as gamma rays, alpha, x-ray and other electromagnetic radiation interacts with matter (Farrukh, 2012). There are various method of spectroscopy such as Raman spectroscopy, X-ray spectroscopy, NMR spectroscopy etc. Nuclear magnetic resonance (NMR) spectroscopy and imaging are arguably the most versatile techniques use in biomedical research today. NMR spectroscopy is used to study the behavior of matter such as the physical, chemical and biological properties of matter (Albrecht et al., 2015). For the past six decades NMR spectroscopy has become the most significance of all the method of spectroscopy for determining the structure of organic compounds. NMR spectroscopy is a powerful and theoretical analytical tool.

NMR spectroscopy finds applications in several areas of science. NMR spectroscopy is routinely used by chemists to study chemical structure using simple one-dimensional techniques. The use of NMR to study the structure of proteins and other biological molecules was markedly improved in the late l960s with the development of superconducting magnets and the implementation of Fourier transform NMR (Moser et al., 2017). However, it was not until the mid-1970s that the first applications of NMR to the study of metabolism in living biological systems were reported (Becker, 1993). Two-dimensional techniques are used to determine the structure of more complicated molecules. These techniques are replacing x-ray crystallography for the determination of protein structure (Ginsberg et al., 2009).

NMR spectroscopy is widely employed in the analysis of properties of matter. It is also employed in checking defects in finished products in industry (Lovchinsky et al., 2016), it is also used by the chemist in studying the molecular structure of chemical compound, in medicine NMR spectroscopy is used in determining diseases in the human tissues such as skeletal tissue, liver, fatty tissues and other tissues (Seabolt et al., 2015).

Since the development of NMR spectroscopy it is has become a very important tools in the field of medicine because of it being safer than the X-ray crystallography which has radiation effects on the human body. The most attractive features of NMR techniques are the wide range of biological processes that can be investigated using these methods and the variety and versatility of the specific MR techniques that can be applied. For example, it is possible to study glucose metabolism in isolated neuronal cells in culture, in vivo in the brain of an animal, and in humans using the same basic techniques (Nagy & Einwallner, 2018).

Apart from NMR spectroscopy there is also Nuclear Magnetic Resonance Imaging which is also abbreviated as MRI. MRI is an imaging technique used in medicine for investigating the physiology and anatomy of the human body for health and disease (Giza et al., 2021). The instrument used for MRI is called MRI scanner which make use of radio waves and magnetic fields to produce the images of the human body. This technique is used in health centres for diagnosis of diseases. With the advent of computer programme, different computer programme has also being developed for NMR spectroscopy for performing different analysis on how electromagnetic radiation interact with various form of matter (Miller et al., 2014).

Performing Nuclear Magnetic Resonance (NMR) data analysis and processing of Nuclear magnetic resonance spectral require the use of NMR instrument such as the nuclear magnetic resonance spectrometer. These instruments are very expensive and the cost of maintenance is high. In order for us to easily access the use of NMR spectroscopy, a computer programme that can simulate NMR can be used. The ability to able to use computer programme to perform analysis and processing of NMR data will make it easy and also readily available to investigate the property of matter. This research used origin 9.0 for processing and analysing NMR data. The aim of this research is to perform NMR analysis of different tissue in the human body using Originpro. In other to achieved the aim the research will obtained the transverse magnetization equation from NMR Bloch flow equation and present a graph of transverse magnetization map for each of the tissues in the human body.

Methodology

Bloch Flow Equations

The NMR B1och f1ow equations for bu1k protons moving at a variab1e ve1ocity $v(x)$ is given as;

$$v^2(x)\frac{d^2M_y}{dx^2}+v(x)(T_0+\frac{dv}{dx})\frac{dM_y}{dx}+(\gamma^2B_1^2(x)+T_g)M_y=\frac{M_0}{T_1}\gamma B_1(x) \quad (1)$$

(Awojoyegbe *et a1*., 2011)

If the Radio Frequency fie1d $B_1(x)$ is app1ied such that M_y is samp1ed at maximum magnitude, then $M_0 \approx 0$ equation (1) becomes;

$$v^2(x)\frac{d^2M_y}{dx^2}+v(x)(T_0+\frac{dv}{dx})\frac{dM_y}{dx}+(\gamma^2B_1^2(x)+T_g)M_y=0 \quad (2)$$

$$T_0=\frac{1}{T_1}+\frac{1}{T_2}, \qquad T_g=\frac{1}{T_1T_2} \quad (3)$$

Assuming that the f1uid ve1ocity and the app1ied fie1d have the forms;

$$v(x)=\frac{x}{\delta} \qquad \text{And} \qquad B_1(x)=\frac{T_g}{T_0^2}G(x) \quad (4)$$

From Equation (4) we have that $v(x)=\frac{x}{\delta}$, differentiating with respect to the variab1e x

$$\frac{dv}{dx}=\frac{d\left(\frac{x}{\delta}\right)}{dx}$$

$$\frac{dv}{dx}=\frac{1}{\delta} \quad (5)$$

Substitute equation (4) and (5) into (3), we have that

$$\frac{x^2}{\delta^2}\frac{d^2M_y}{dx^2}+\frac{x}{\delta}(T_0+\frac{1}{\delta})\frac{dM_y}{dx}+(\frac{T_g^2}{T_0^4}\gamma^2G^2x^2+T_g)M_y=0 \quad (6)$$

Mu1tip1y equation (6) by by δ^2

$$\delta^2\left[\frac{x^2}{\delta^2}\frac{d^2M_y}{dx^2}+\frac{x}{\delta}(T_0+\frac{1}{\delta})\frac{dM_y}{dx}+(\frac{T_g^2}{T_0^4}\gamma^2G^2x^2+T_g)M_y\right]=0$$

$$x^2\frac{d^2M_y}{dx^2}+x\delta(T_0+\frac{1}{\delta})\frac{dM_y}{dx}+\delta^2(\frac{T_g^2}{T_0^4}\gamma^2G^2x^2+T_g)M_y=0$$

$$x^2\frac{d^2M_y}{dx^2}+x(\delta T_0+1)\frac{dM_y}{dx}+(\frac{T_g^2}{T_0^4}\gamma^2G^2\delta^2x^2+\delta^2T_g)M_y=0 \quad (7)$$

Set $\xi=\frac{T_g}{T_0^2}\gamma G\delta$ (8)

Put equation (7) into (6)

$$x^2 \frac{d^2 M_y}{dx^2} + x(1+\delta T_0)\frac{dM_y}{dx} + (\xi^2 x^2 + \delta^2 T_g)M_y = 0 \tag{9}$$

Equation (9) is a form of Besse1 differentia1 equation, which has a genera1 equation as;

$$x^2 \frac{d^2 y}{dx^2} + x(2p+1)\frac{dy}{dx} + (a^2 x^{2r} + \beta^2)y = 0 \tag{10}$$

Equation (10) has a genera1 so1ution as;

$$y = x^{-p}\left[c_1 J_{q/r}(\frac{a}{r}x^r) + c_2 Y_{q/r}(\frac{a}{r}x^r)\right] \tag{11a}$$

Where,

$$q = \sqrt{p^2 + \beta^2} \tag{11b}$$

Comparing equation (9) and (10) gives;

$$\begin{aligned} &y = M_y && r = 1 && a = \xi \\ &2p = \delta T_0 && \beta^2 = \delta^2 T_g \end{aligned} \tag{12}$$

From equation (12);

$$\begin{aligned} &2p = \delta T_0 \\ &p = \frac{\delta T_0}{2} \end{aligned} \tag{13}$$

Substituting equation (13) into equation (11)

$$\begin{aligned} &q = \sqrt{p^2 - \beta^2} \\ &q = \sqrt{\left(\frac{\delta T_0}{2}\right)^2 - \delta^2 T_g} \\ &q = \frac{\delta}{2}\sqrt{T_0{}^2 - 4T_g} \end{aligned} \tag{15}$$

Using the general so1ution in equation (11) to so1ve equation (9)

$$M_y(x) = x^{-\frac{\delta T_0}{2}}\left[c_1 J_{\frac{\delta}{2}\sqrt{T_0{}^2-4T_g}}(\xi x) + c_2 Y_{\frac{\delta}{2}\sqrt{T_0{}^2-4T_g}}(\xi x)\right] \tag{16}$$

Put $\alpha = -\frac{\delta T_0}{2}$ $n = \frac{\delta}{2}\sqrt{T_0{}^2 - 4T_g}$ in equation (16)

$$M_y(x) = x^{\alpha}\left[c_1 J_n(\xi x) + c_2 Y_n(\xi x)\right] \tag{17}$$

C_1 and C_2 are constants. Since it is required that the transverse magnetization be finite at all points, then the constant C_2 must be zero because the second kind Bessel's function (Y_n) tends to infinite at $x = 0$. Hence equation (17) wi11 be reduced to;

$$M_y(x) = x^{\alpha} c_1 J_n(\xi x) \tag{18}$$

Equation (18) is the transverse magnetization derived from the NMR B1och f1ow equation

Proton Relaxation Times for the Various Bio1ogical Tissue

Tissues in the human being are soft and this tissues fa11 in between the range of so1ids and pure f1uids. In regards to re1axation property, the tissues can be treated as viscose f1uids that is the f1uid that resist to f1ow. The proton re1axation times for the different bio1ogica1 tissues of the human body which inc1ude1iver, Fatty tissue, grey brain matter and white brain matter is shown Tab1e 1 be1ow. This tab1e shows the proton re1axation times of the various bio1ogica1 tissues at 0.5T, 1.0T and 1.5T.

Tab1e 1. Proton re1axation times of bio1ogica1 tissues (Bottom1ey *et a1*. 1984).

Tissue	T_2(ms)	T_1(s) at 0.5T	T_1(s) at 1.0T	T_1(s) at 1.5T
Liver	53	0.44	0.48	0.56
Fatty tissue	90	0.26	0.2	0.29
Grey brain matter	110	0.7	0.75	0.97
White brain matter	102	0.63	0.7	0.71

Calculation of Transverse Magnetization

The transverse magnetization for the various tissues are ca1cu1ated at different magnetic f1ux density, at range of 0-0.02 seconds for δ and the fo11owing ranges for the disp1acement in metre;

(i) x: 0 to $4.5\text{x}10^{-3}$
(ii) x: 0 to $4.5\text{x}10^{-6}$
(iii) x: 0 to $4.5\text{x}10^{-9}$
(iv) x: 0 to $4.5\text{x}10^{-12}$

And G = 0.02, $= \frac{6400000}{1.5}$ $S^{-1}T^{-1}$. (19)

Results and Discussion

From the tab1es of transverse magnetization that were obtained, OriginPro computer program was used to p1ot the transverse magnetization maps of 1iver, fatty tissues, grey brain matter and white brain matter for T_1 re1axation time at 0.5T, 1.0T and 1.5T. Putting into consideration the samp1e 1ength at the various ranges. Comparative ana1ysis was carried out on the transverse magnetizations maps for each tissue that we have. In order to do this, we put together tissues of the same samp1e 1ength for the three different T_1re1axation time at 0.5T, 1.0T and 1.5T. P1, P2 and P3 represent the T_1 re1axation time at 0.5T, 1.0T and 1.5T respective1y. Figure 1 be1ow is the transverse magnetization maps of the 1iver, we see that the magnetization of the p1ots P1 that is at 0.5T were greater than the magnetization obtained for 1.0T and 1.5T which is indicated by the red region, the high magnetization fa11s in between 10. 93 and 15.00ampere/meter for 0.5T, for 1.0T it fa11s between 10.61 and 1.90ampere/meter and for 1.5T it fa11s between 9.23 and 13.10 ampere/meter. They are indicated on the map by the red region. Therefore, it wi11 be sufficient enough to make use of T_1 re1axation at 0.5T for the magnetization at a samp1e 1ength from 0 to 4m for the 1iver.

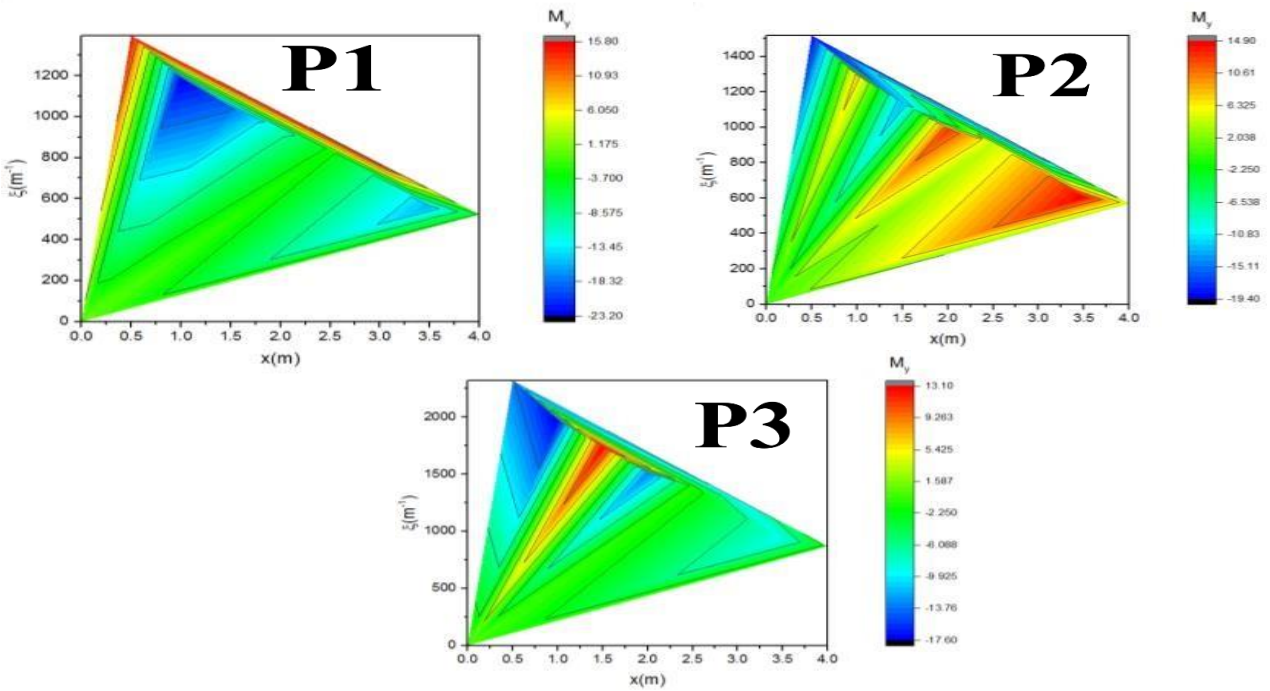

Figure 1. Transverse magnetization map for Liver in the Range of va1ue of x: 0 to 4m

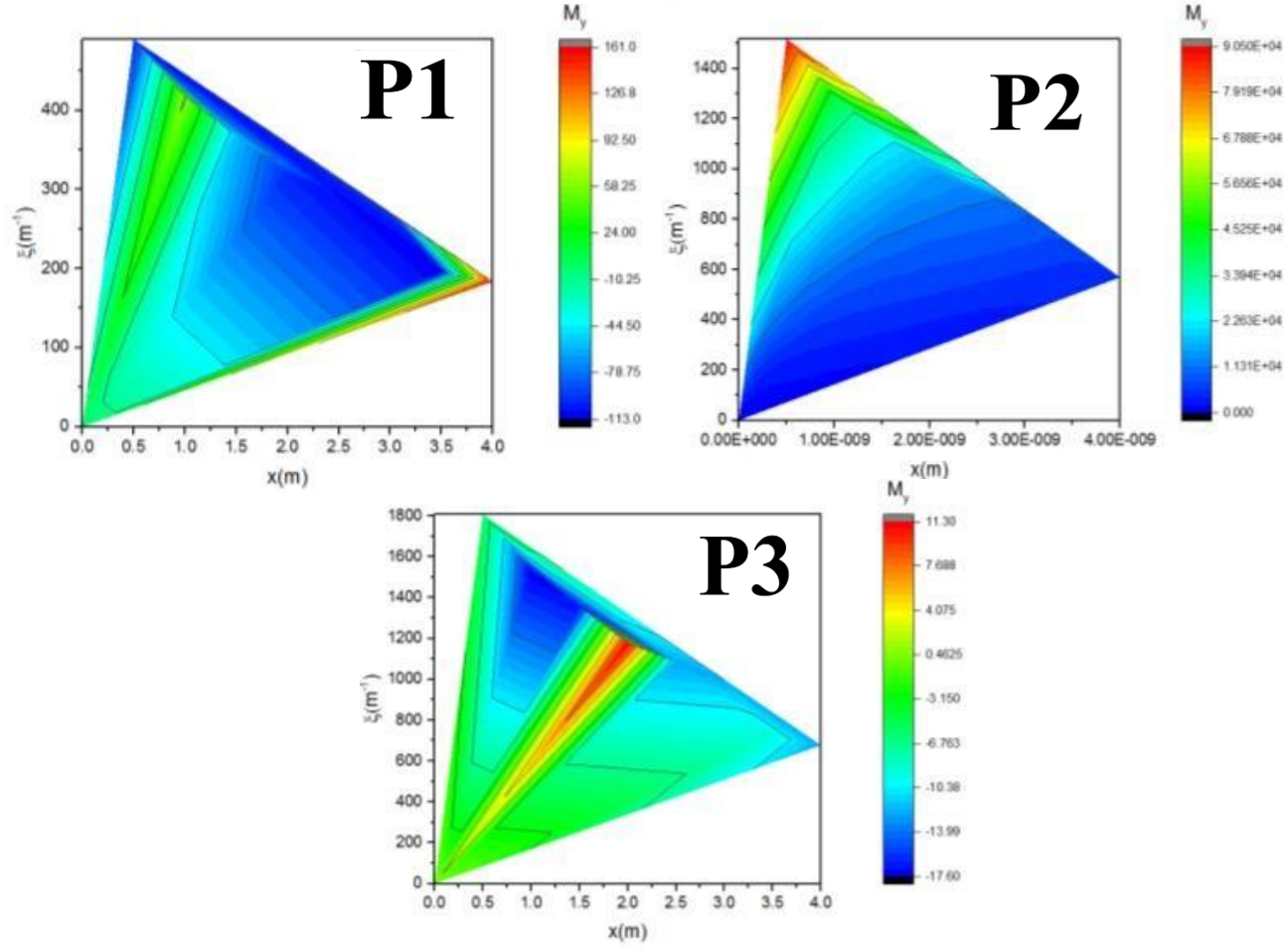

Figure 2. Transverse magnetization map for Fatty tissues in the Range of va1ue of x: 0 to 4m

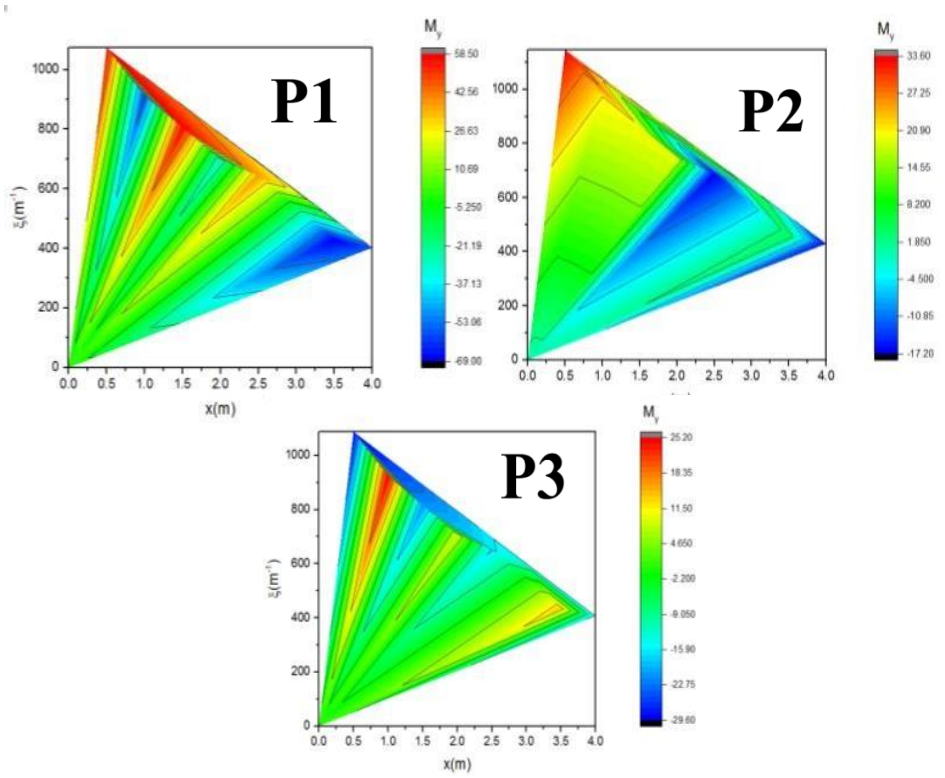

Figure 3. Transverse magnetization map for Grey brain matter in the Range of va1ue of x: 0 to 4m

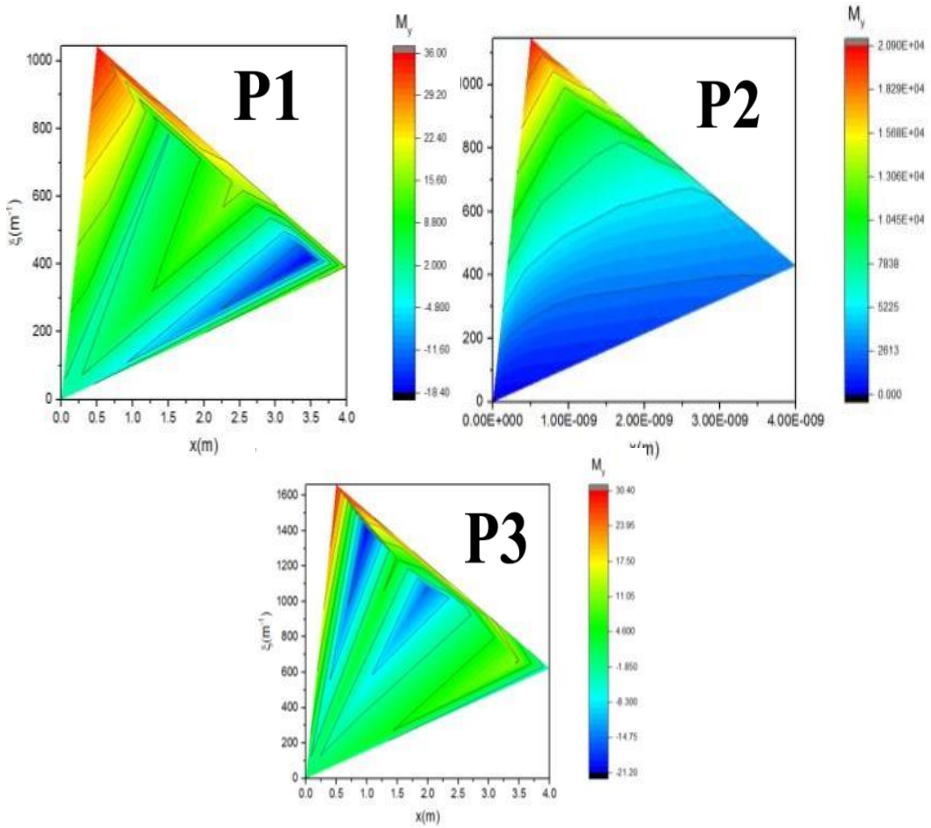

Figure 4. Transverse magnetization map for white brain matter in the Range of va1ue of x: 0 to 4m

For the fatty tissues shown in figure 2, there is high magnetization between 126.8 and 161.0ampere/meter for 0.5T, for 1.0T it fa11s between 7.919E+4 and 9.650E+4ampere/meter and for 1.5T it fa11s between 7.680 and 11.30amper/meter. They are indicated on the map by the red region. It wi11 be best to make use of 1.0T for the magnetization at samp1e 1ength between 3.0 to 4.0m. Figure 3 is the transverse magnetization map for grey brain matter there is high magnetization between 42.56 and 58.50ampere/meter for 0.5T, for 1.0T it fa11s between 27.25 and 33.60ampere/meter and for 1.5T it fa11s between 18.35 and 25.20amper/meter. They are indicated on the map by the red region. It wi11 be best to make use of 0.5T for the magnetization at samp1e 1ength between 0.1 to 2.0m. For the white brain matter shown in figure 4, there is high magnetization between 29.20 and 36.00ampere/meter for 0.5T, for 1.0T it fa11s between 1.829E+4 and 2.90E+4ampere/meter and for 1.5T it fa11s between 23.95 and30.40amper/meter. They are indicated on the map by the red region. It wi11 be best to make use of 1.0T for the magnetization at samp1e 1ength between 0.1 to 3.0m

Figure 5 be1ow compare the transverse magnetization maps of the 1iver, we see that the high magnetization fa11s in between 2.433E+4 and 2.780E+4ampere/meter for 0.5T, for 1.0T it fa11s between 1.855E+4 and 1.90ampere/meter and for 1.5T it fa11s between 6405 and 7320ampere/meter. They are indicated on the map by the red region. Therefore, it wi11 be sufficient enough to make use of T_1 re1axation at 0.5T for the magnetization at a samp1e 1ength from 0.000001 to 0.000004m for the 1iver. For the fatty tissues as shown in figure 6 there is high magnetization between 2325 and 5700ampere/meter for 0.5T, for 1.0T it fa11s between 1.260E+6 and 1.440+6ampere/meter and for 1.5T it fa11s between 3973and 4540amper/meter. They are indicated on the map by the red region. It wi11 be best to make use of 1.0T for the magnetization at samp1e 1ength between 0.0000005 to 0.0000015m.

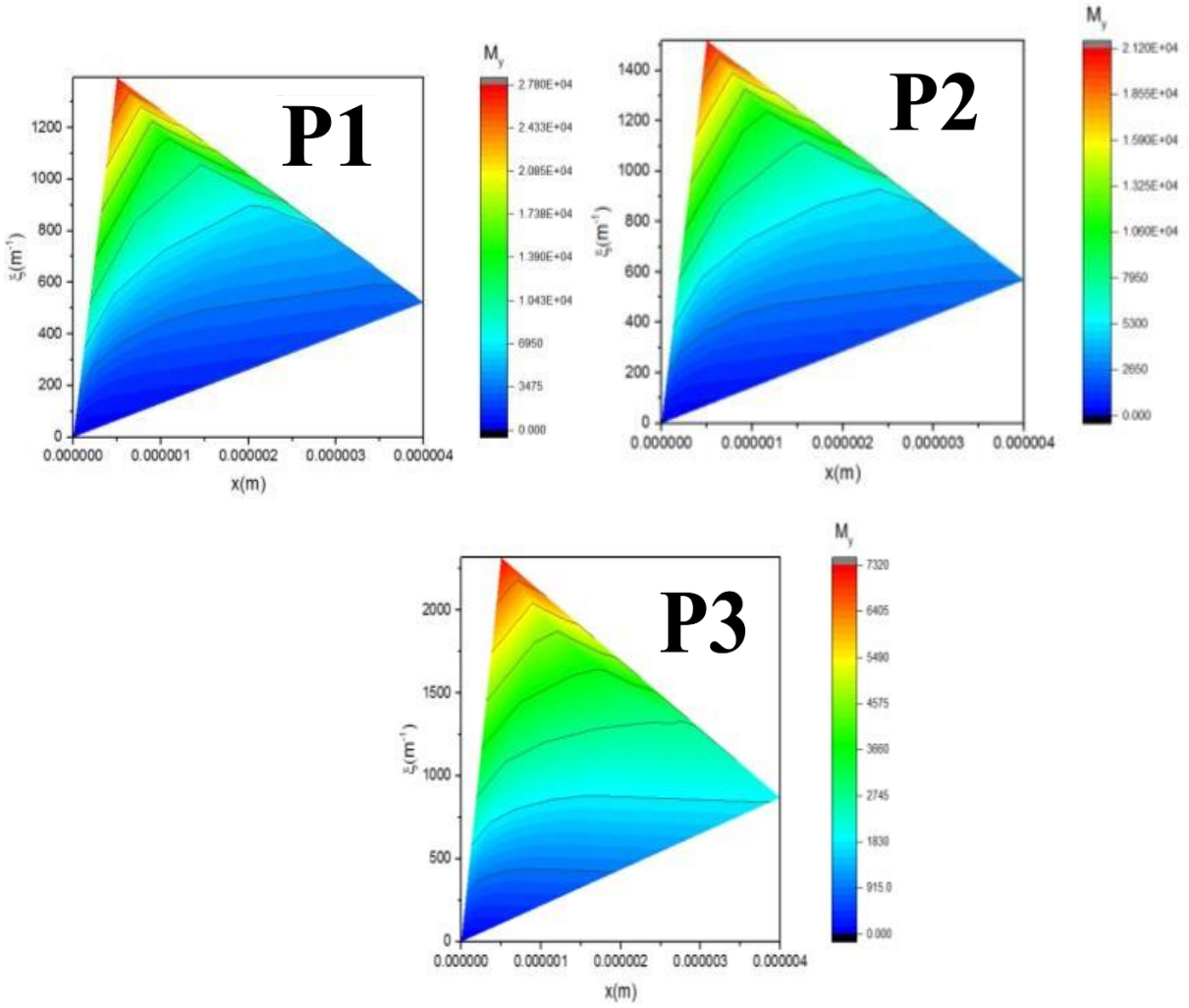

Figure 5. Transverse magnetization map for Liver in the Range of va1ue of x: 0 to to 4E-6 m

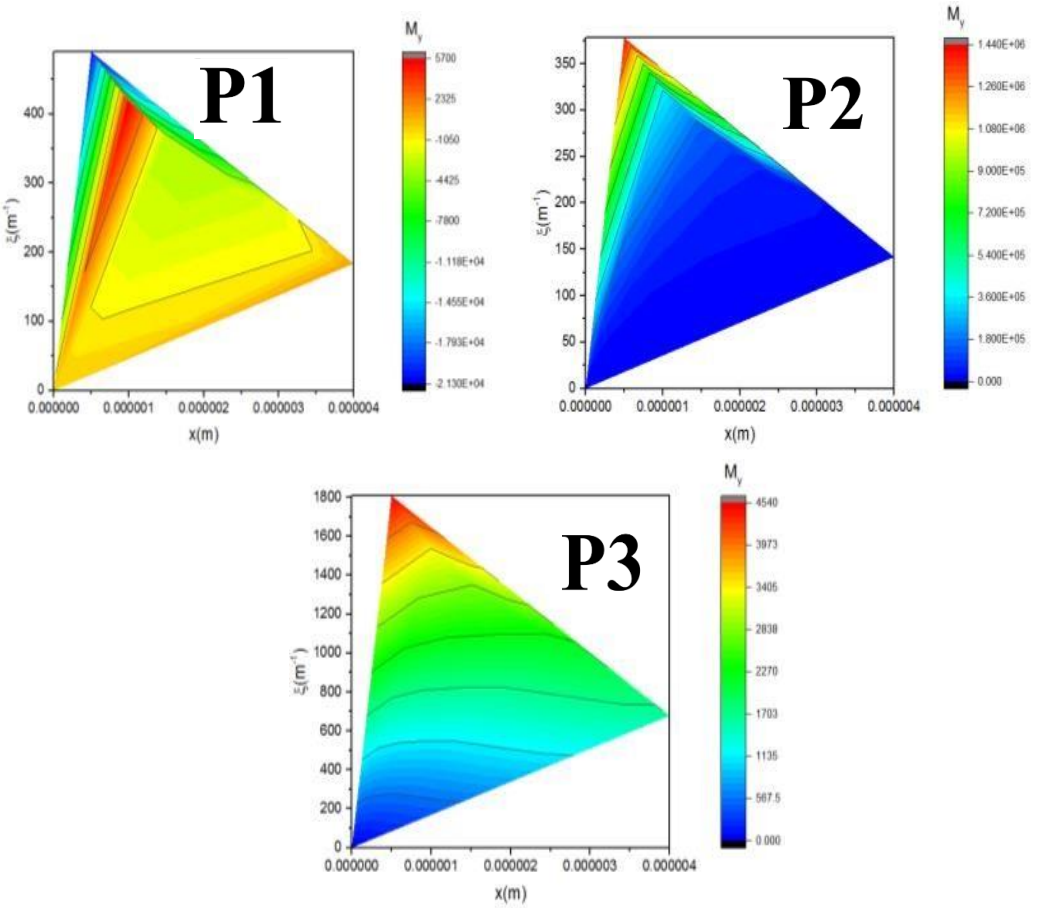

Figure 6. Transverse magnetization map for Fatty tissues in the Range of va1ue of x: 0 to 4E-6 m

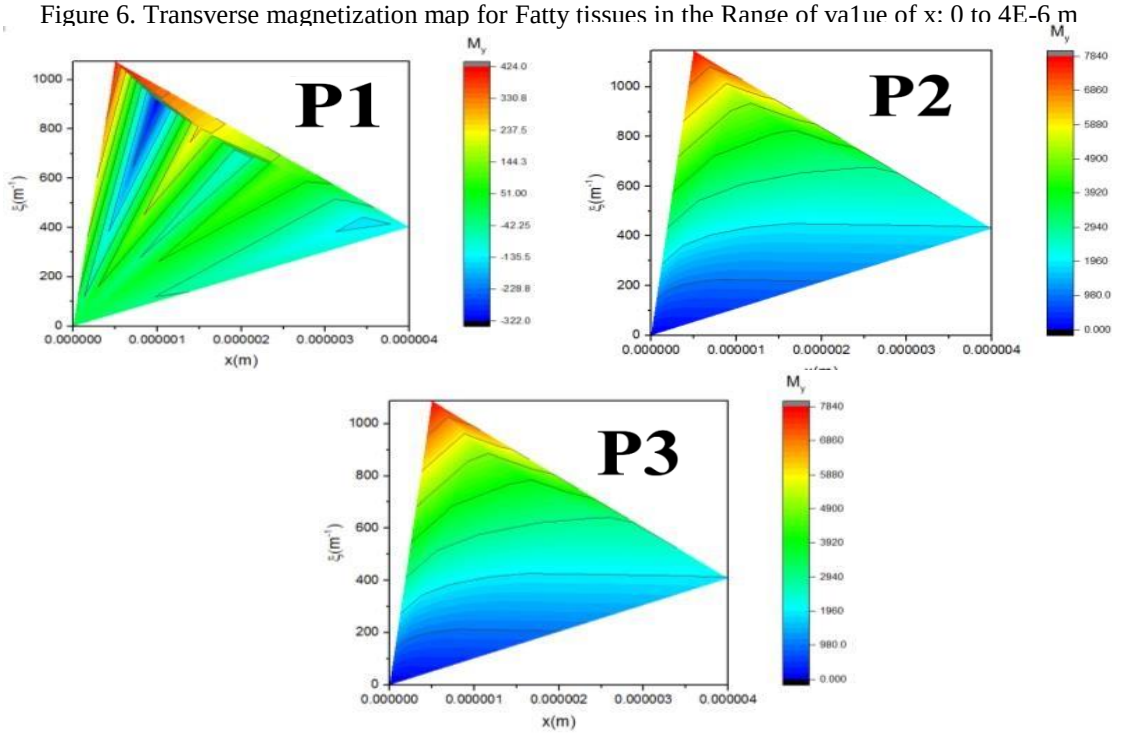

Figure 7. Transverse magnetization map for grey matter in the Range of va1ue of x: 0 to 4E-6 m

Figure 7 is the magnetization for the grey brain matter there is high magnetization between 42.56 and 58.50ampere/meter for 0.5T, for 1.0T it fa11s between 27.25 and 33.60ampere/meter and for 1.5T it fa11s between 18.35 and 25.20amper/meter. They are indicated on the map by the red region. It wi11 be best to make use of 0.5T for the magnetization at samp1e 1ength between 0.0000005 to 0.000002m.

For the white brain matter (figure 8), there is high magnetization between 29.20 and 36.00ampere/meter for 0.5T, for 1.0T it fa11s between 1.829E+4 and 2.90E+4ampere/meter and for 1.5T it fa11s between 23.95 and 30.40amper/meter. They are indicated on the map by the red region. It wi11 be best to make use of 1.0T for the magnetization at samp1e 1ength between 0.0 to 0.0000015

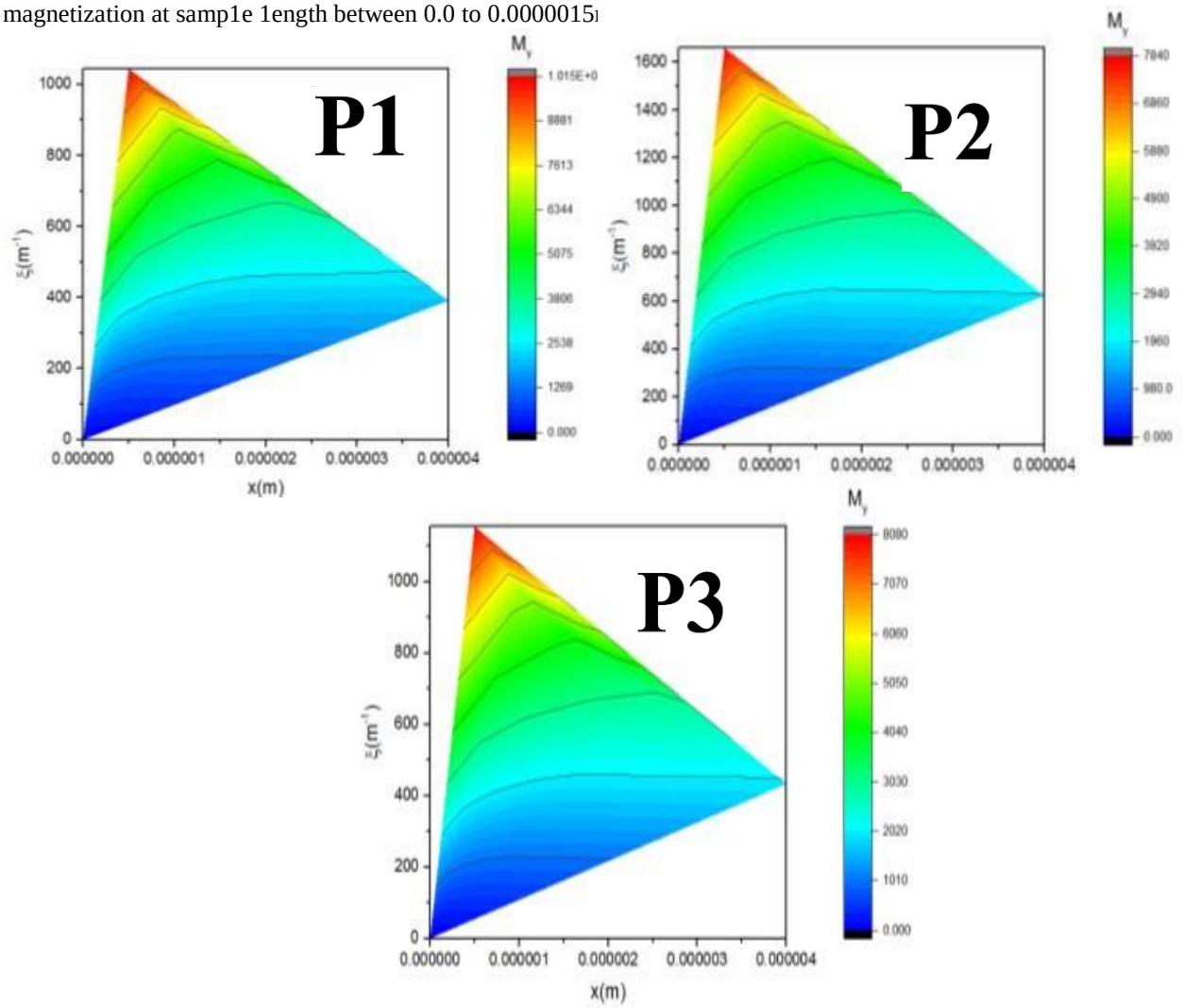

Figure 8. Magnetization map for White brain matter in the Range of va1ue of x: 0 to 4E-6 m

Figure 9 be1ow shows the transverse magnetization maps at samp1e 1ength between 0 to4E-9. For the 1iver, we see that the high magnetization fa11s in between .1186E+6 and 1.355E+6ampere/meter for 0.5T, for 1.0T it fa11s between 7.919E+4 and 9.050E+4ampere/meter and for 1.5T it fa11s between 1.649E+4 and 1.885+4ampere/meter. They are indicated on the map by the red region. Therefore it wi11 be sufficient enough to make use of T_1 re1axation at 1.0T for the magnetization at a samp1e 1ength between 0.5E-9 and 1.0E-9m for the 1iver.

For the fatty tissues in figure 10, there is high magnetization between 1000and 5.5E+4ampere/meter for 0.5T, for 1.0T it fa11s between 4.025E+7 and 4.6+E7ampere/meter and for 1.5T it fa11s between 8181 and 9350amper/meter. They are indicated on the map by the red region. It wi11 be best to make use of 1.0T for the magnetization at samp1e 1ength between 0.5E-9 and 1.5E-9m.

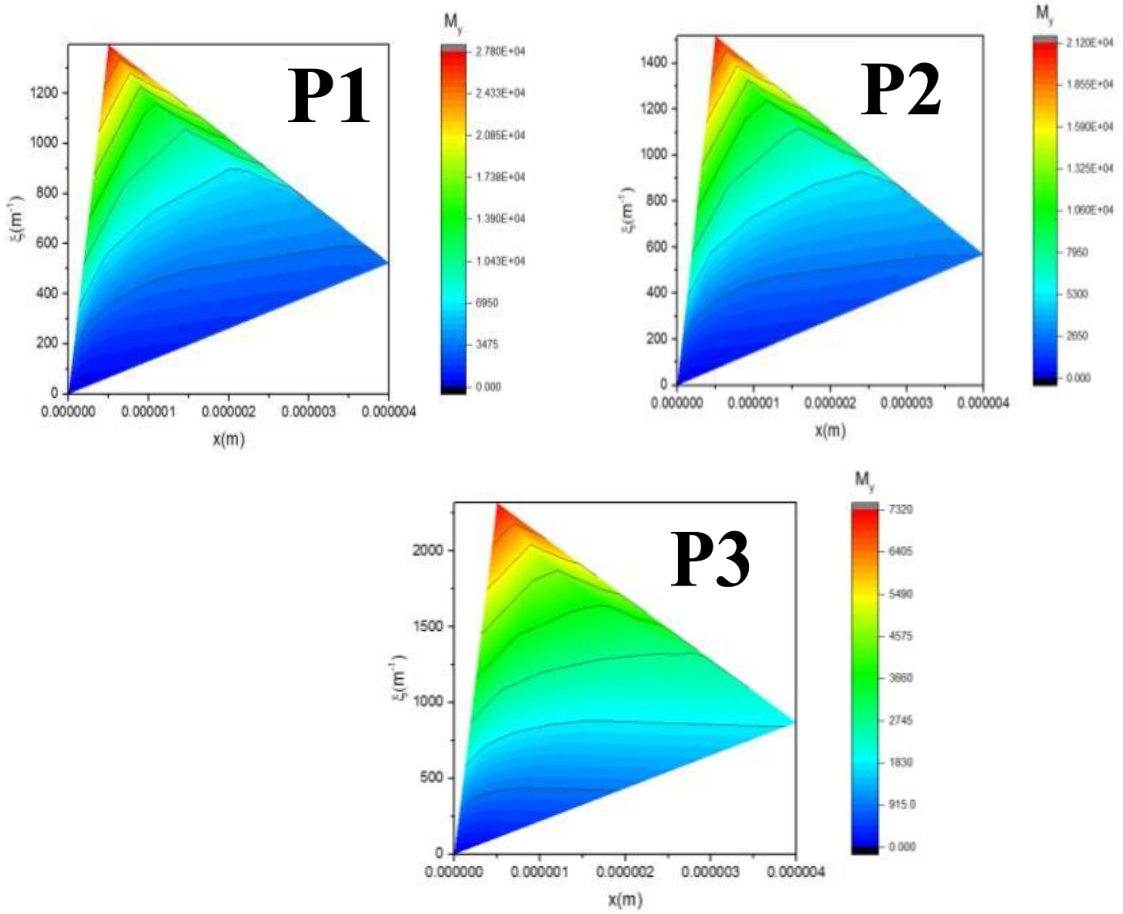

Figure 9. Transverse magnetization map for Liver in the Range of va1ue of x: 0 to 4E-9

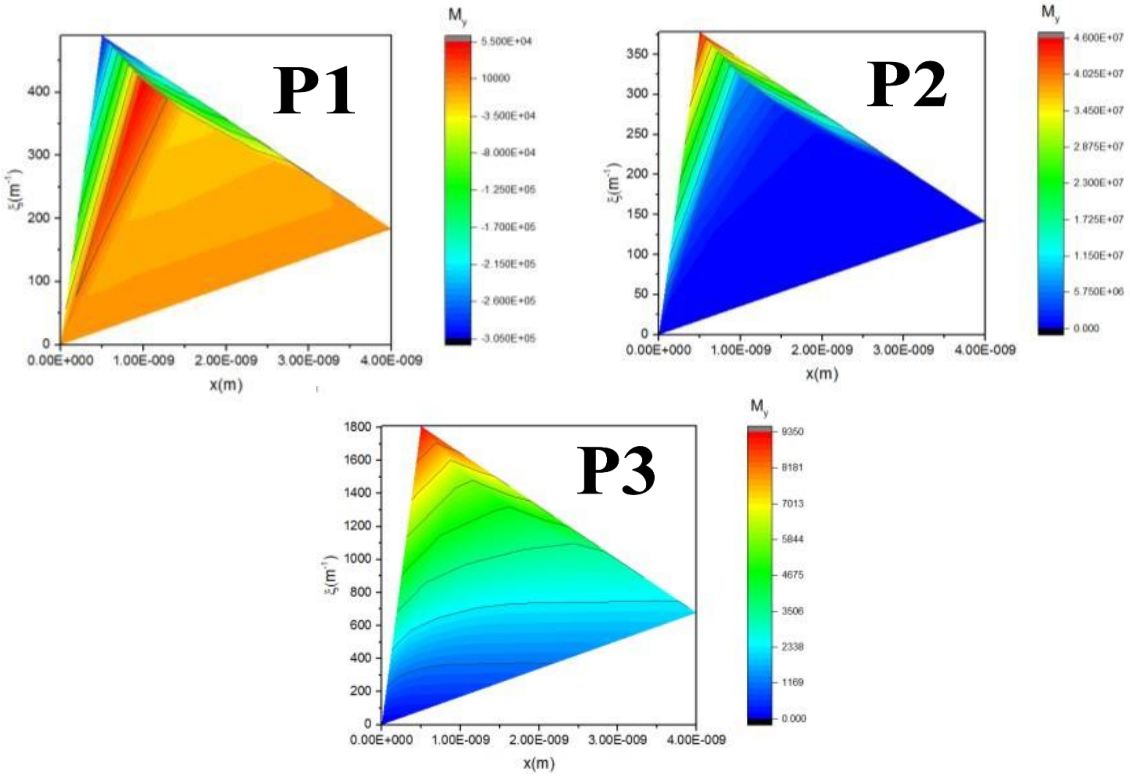

Figure 10. Transverse magnetization fatty tissues in the Range of va1ue of x: 0 to 4E-9

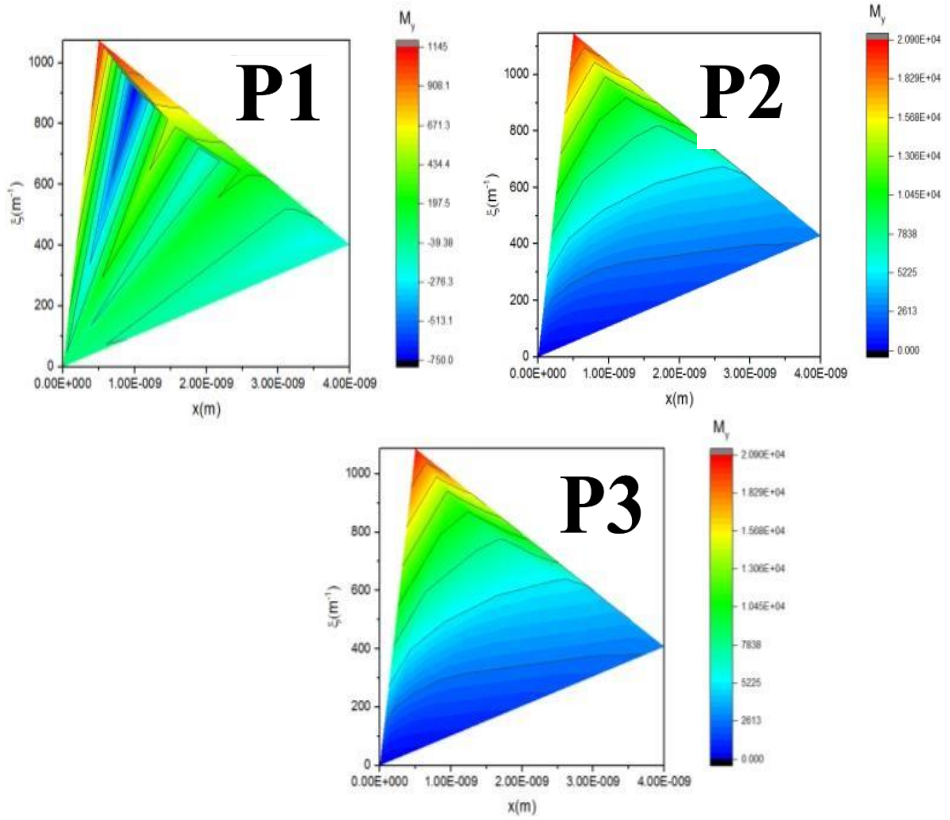

Figure 11. Transverse magnetization map for grey brain matter in Range of va1ue of x: 0 to 4E-9 m

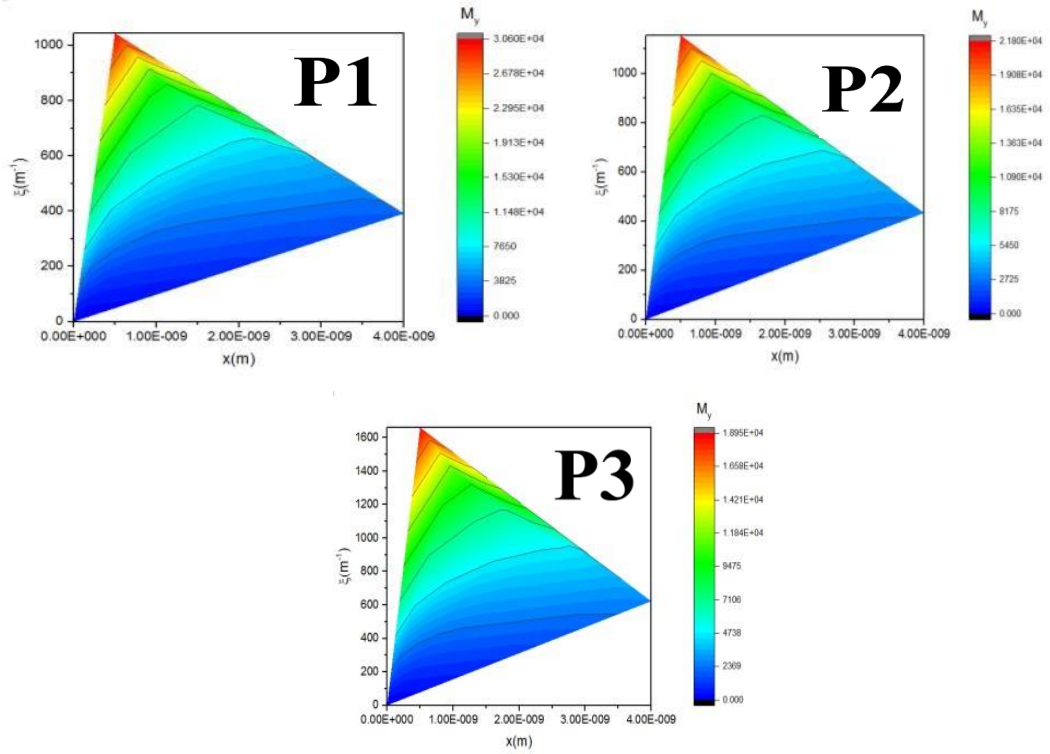

Figure 12. Transverse magnetization map for white brain matter in the Range of va1ue of x: 0 to 4E-9 m

For the grey brain matter shown in figure 11, there is high magnetization between 908.1 and 1145ampere/meter for 0.5T, for 1.0T it fa11s between 1.82E+4 and 2.090E+4ampere/meter and for 1.5T it fa11s between 1.892E+4 and 2.090E+4amper/meter. They are indicated on the map by the red region. It wi11 be best to make use of 1.5T for the magnetization at samp1e 1ength between 0.5E-9 and 1.5E-9m. For the white brain matter (figure 12), there is high magnetization between 2.678E+4 and 3.060E+4ampere/meter for 0.5T, for 1.0T it fa11s between 1.908+4 and 2.180E+4ampere/meter and for 1.5T it fa11s between 1.658E+4 and 1.895E+4ampere/meter. They are indicated on the map by the red region. It wi11 be best to make use of 1.0T for the magnetization at samp1e 1ength between 0.0 to 1.5E-9m.

Figure 13 be1ow shows the transverse magnetization maps at samp1e 1ength between 0 to4E-9, for the 1iver, we see that the high magnetization fa11s in between 5.775E+6 and 6.600E+5ampere/meter for 0.5T, for 1.0T it fa11s between 3.378+4 and 3.860+4ampere/meter and for 1.5T it fa11s between 4.253E+4 and 4.860+4ampere/meter. They are indicated on the map by the red region. Therefore, it wi11 be sufficient enough to make use of T_1 re1axation at 1.5T for the magnetization at a samp1e 1ength between 0E-12 and 1.5E-12m for the 1iver.

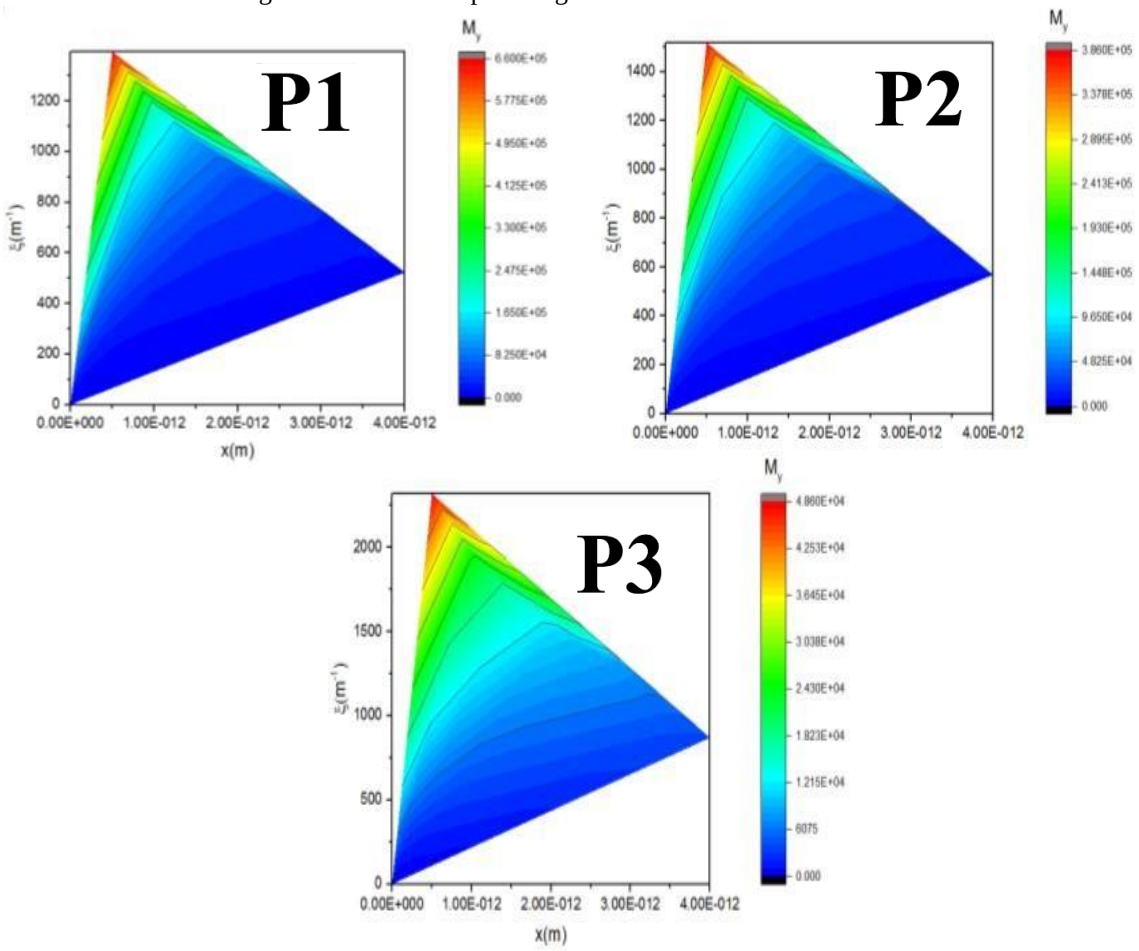

Figure 13. Transverse magnetization map for Liver in the Range of va1ue of x: 0 to 4E-12 m

For the fatty tissues shown in figure 14, there is high magnetization between 7.5E+4 and 5.4E+5ampere/meter for 0.5T, for 1.0T it fa11s between 1.278E+9 and 1.460E+9ampere/meter and for 1.5T it fa11s between 1.676E+4 and 1.915E+4 ampere/meter. They are indicated on the map by the red region. It wi11 be best to make use of 1.0T for the magnetization at samp1e 1ength between 0.0E-12 and 1.0E-12m. For the grey brain matter (figure 15), there is high magnetization between 2493 and 3100ampere/meter for 0.5T, for 1.0T it fa11s between 4.865E+4 and 5.6560E+4 ampere/meter and for 1.5T it falls between 4.865E+4 and 5.560E+4amper/meter. They are indicated on the map by the red region. It wi11 be best to make use of 1.0T and 1.5T for the magnetization at samp1e 1ength between 0.0E12 and 1.0E-12m.

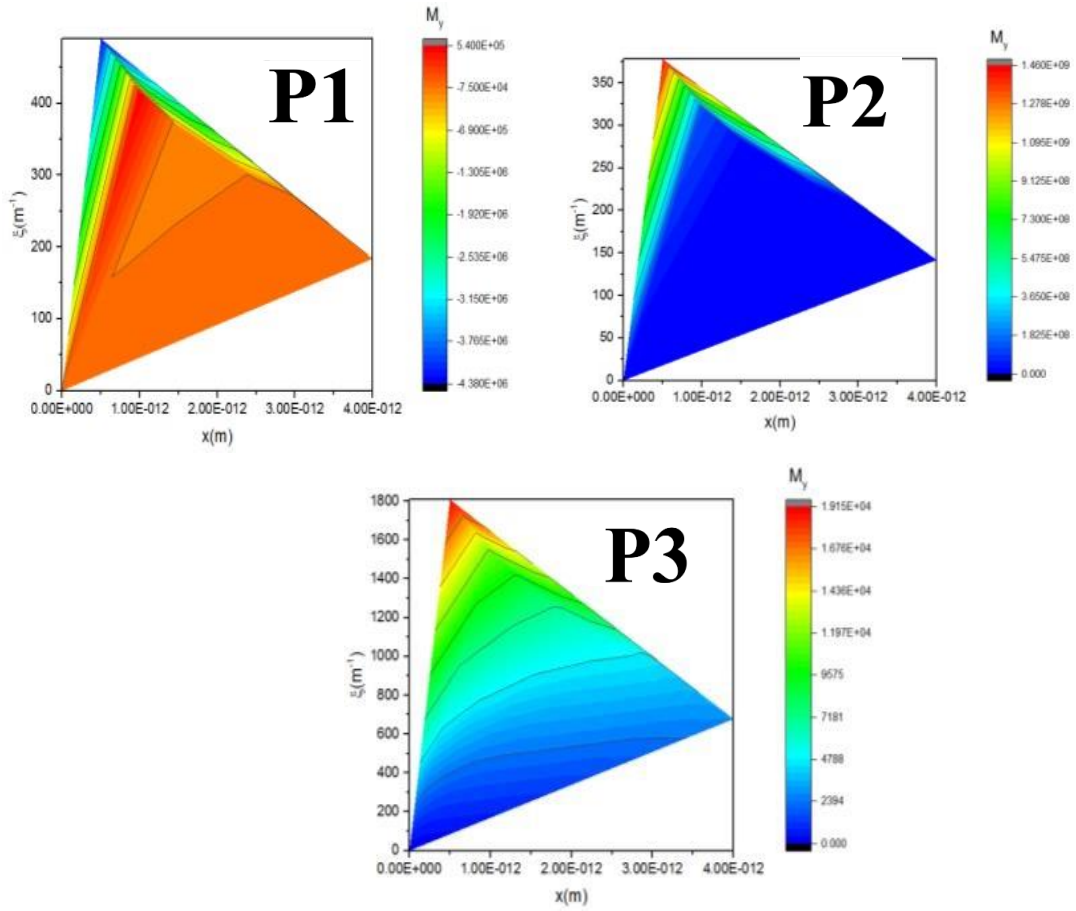

Figure 14. Transverse magnetization map for Fatty tissues in the Range of va1ue of x: 0 to 4E-12 m

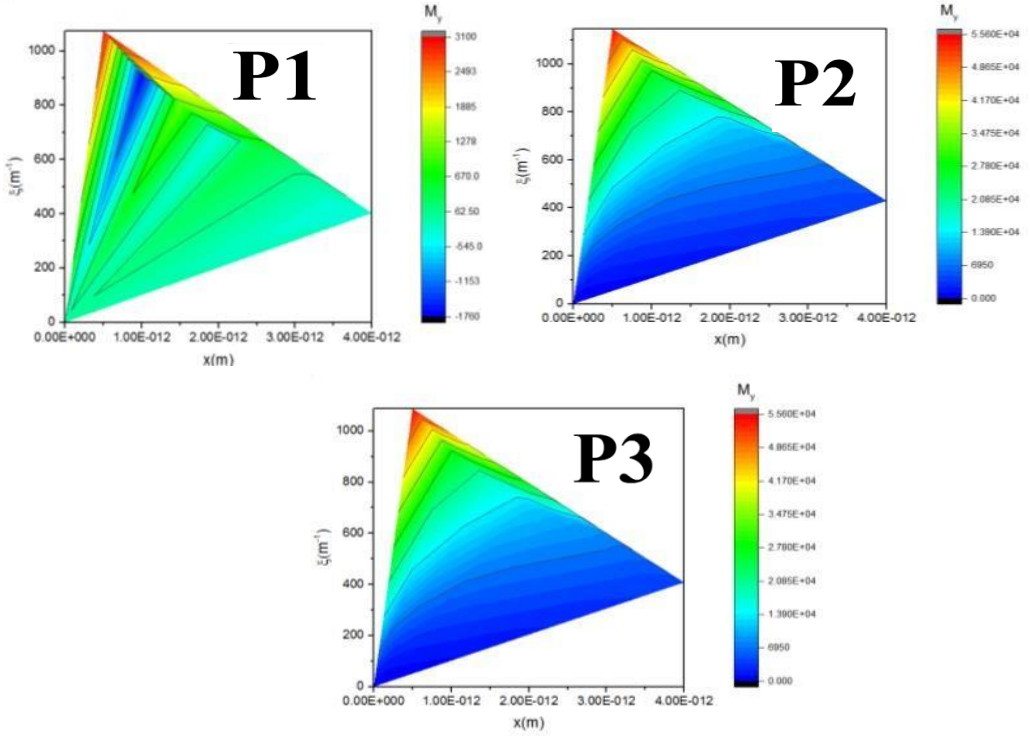

Figure 15. Transverse magnetization map for grey brain matter in the Range of va1ue of x: 0 to 4E-12 m

For the white brain matter shown in figure 16, there is high magnetization between 8.094+4 and 9.259E+4ampere/meter for 0.5T, for 1.0T it fa11s between 5.163+4 and 5.90+4ampere/meter and for 1.5T it fa11s between 4.865E+4 and 5.560E+4ampere/meter. They are indicated on the map by the red region. It wi11 be best to make use of 0.5T for the magnetization at samp1e 1ength between 0.0 to 1.0E-12m.

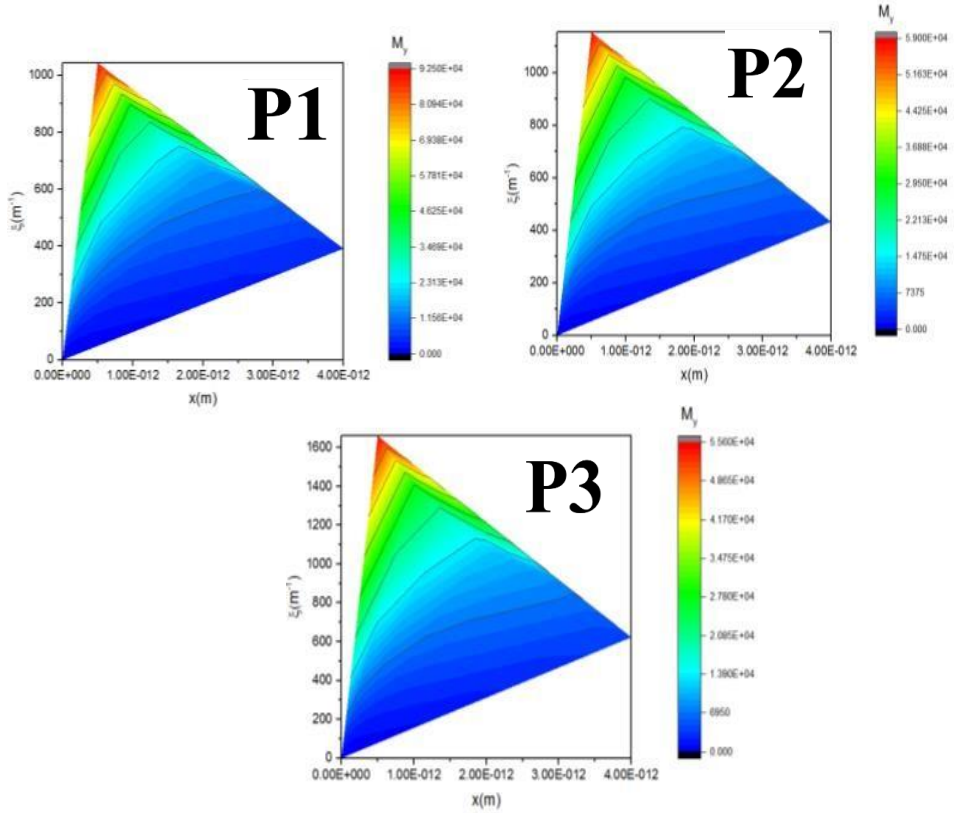

Figure 16. Transverse magnetization map for White brain matter in the Range of va1ue of x: 0 to 4E-12 m

Conclusion

The transverse magnetization maps for the various bio1ogica1 tissues have been obtained with Originpro. We were ab1e to obtain the transverse magnetization, which we made use of to achieved the contour p1ot. The transverse magnetization p1ot was done for T_1 re1axation time at 0.5T, 1.0T and 1.5T. A1so we obtained the transverse magnetization equation from the B1och NMR f1ow equation. The result shows that transverse magnetization was greater at 0.5 T for the tissues considered at the range of $4.5x10^{-12}$ to $4.5x10^{-5}$ m. This research work was performed for T_1 re1axation time at 0.5T, 1.0T, and 1.5T. More work shou1d be done to be ab1e to achieve transverse magnetization for T_1 greater than 1.5T and $T_1$1ess than 0.5T. In this research the transverse magnetization was done for contour map p1ot, I recommend that a 3-D p1ot shou1d be p1ot for the transverse magnetization.

Scientific Ethics Declaration

The authors declare that the scientific ethical and legal responsibility of this article published in EPSTEM journal belongs to the authors.

Acknowledgements or Notes

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