

Analytical Solution to Diffusion-Advection Equation in Spherical Coordinate Based on the Fundamental Bloch NMR Flow Equations

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Abstract A general solution for transverse magnetization, the nuclear magnetic resonance (NMR) signals for diffusion-advection equation with spatially varying velocity and diffusion coefficients, which is based on the fundamental Bloch NMR flow equations, was obtained using the method of separation of variable. It assumed that the velocity component is proportional to the coordinate and that the diffusion coefficient is proportional to the square of the corresponding component. There is a simple transformation which reduces the spatially variable equation to a constant coefficient. After some assumptions, the 3-D equation degenerates to a 2-D problem. The solution to this equation is useful in describing physical phenomenon such as transport of materials in a fluid. The result obtained in this study can have applications in functional magnetic resonance imaging (fMRI) with more accurate information.

Keywords NMR diffusion advection equation, Diffusion coefficient, Separation of variable, Magnetic resonance imaging (MRI)

1. Introduction

To investigate the diffusion process of magnetization in a fluid moving at a uniform velocity, v , which is constant in time, we have to take the process of advection into consideration. The equation which describes such a process is known as the advection equation (Awojoyegbe *et.al*, 2010). The advection equation is the partial differential equation that governs the motion of a conserved scalar as it is advected by a known velocity field. It is derived using the scalar's conservation law, together with Gauss's theorem, and taking the infinitesimal limit. The diffusion-advection equation (a differential equation describing the process of diffusion and advection) is obtained by adding the advection operator to the main diffusion equation. In the spherical coordinates, the advection operator is

$$\vec{v} \cdot \nabla = v_r \frac{\partial}{\partial r} + v_\theta \frac{1}{r} \frac{\partial}{\partial \theta} + v_\phi \frac{1}{r \sin \theta} \frac{\partial}{\partial \phi}$$

Where the velocity vector v has components v_r, v_θ , and v_ϕ in the r , θ , and ϕ directions, respectively.

2. The NMR Diffusion Advection Equation

In accordance with Awojoyogbe *et.al* 2010, The NMR diffusion-advection equation with variable coefficient could be obtained from

$$\nabla \cdot (vM_y) + \frac{\partial M_y}{\partial t} = \nabla \cdot (D \nabla M_y) + \frac{F_o}{T_o} \gamma \beta_i(r, t) \quad (r)$$

Where ∇ is the Del operator in the spherical coordinate system.

We have to re-write the advection operator (the first term on the left hand side of Eq. (r)) because this fluid velocity is now spatially dependent. Generally speaking, the advection term for the transverse magnetization is $\nabla \cdot (vM_y)$. After expansion we obtained

$$\nabla \cdot (vM_y) = (\nabla \cdot v)M_y + v \cdot \nabla M_y$$

When the fluid velocity is constant, $\nabla \cdot v = 0$ and then $\nabla \cdot (vM_y) = v \cdot \nabla M_y$ this is similar to a case of incompressible fluid in fluid dynamics.

Since perfusing substances obey the advection equation, the appropriate equation to accurately describe a flow process in a spherical geometry based on equation (r).

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Awojoyobe et al., 2010 is

$$\begin{aligned} & \frac{\partial(v_r M_y)}{\partial r} + \frac{1}{r} \frac{\partial(v_\theta M_y)}{\partial \theta} + \frac{1}{r \sin \theta} \frac{\partial(v_\phi M_y)}{\partial \phi} + \frac{\partial M_y}{\partial t} \\ &= \frac{1}{r^2} \frac{\partial}{\partial r} \left(D_r r^2 \frac{\partial M_y}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left(D_\theta \sin \theta \frac{\partial M_y}{\partial \theta} \right) \\ &+ \frac{1}{r^2 \sin^2 \theta} \frac{\partial}{\partial \phi} \left(D_\phi \frac{\partial M_y}{\partial \phi} \right) + \frac{F_o}{T_o} \gamma \beta_1(r, t) \end{aligned} \quad (1)$$

If the parameters D_r, D_θ, D_ϕ represent the diffusion coefficients, then the equation above is the equation of diffusion of magnetization as the nuclear spins move. The

function $\frac{F_o}{T_o} \gamma \beta_1(r, t)$ is the forcing function, which shows

that the application of radio frequency (RF), β_1 field has an influence on the diffusion of magnetization. It is interesting to note that the dimension of equation above exactly matches that of diffusion coefficient.

In this paper, we are interested in getting the general solution of the equation using the method of separation of variables.

If we define

$$\begin{aligned} v_r &= u_0 r \\ v_\theta &= w_0 \theta \\ v_\phi &= v_0 \phi \end{aligned}$$

and

$$\begin{aligned} D_r &= D_0 u_0^2 r^3 \\ D_\theta &= D_0 w_0^2 \theta^2 \quad (\text{Dada et al., 2010}) \\ D_\phi &= D_0 v_0^2 \phi^2 \end{aligned}$$

Where u_0, v_0, w_0, D_0 are constants (M. Dada. et al., 2010)

In each direction the velocity component has a linear dependence on the coordinates and the corresponding diffusion coefficient has a quadratic dependence on the

coordinates. And if we assume $\frac{\partial}{\partial \phi} = 0$ (E. Danladi et al., 2015) then the equation above reduces to

$$\begin{aligned} & \frac{\partial(v_r M_y)}{\partial r} + \frac{1}{r} \frac{\partial(v_\theta M_y)}{\partial \theta} + \frac{\partial M_y}{\partial t} = \frac{1}{r^2} \frac{\partial}{\partial r} \left(D_r r^2 \frac{\partial M_y}{\partial r} \right) \\ &+ \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left(D_\theta \sin \theta \frac{\partial M_y}{\partial \theta} \right) + \frac{F_o}{T_o} \gamma \beta_1(r, t) \end{aligned} \quad (2)$$

Differentiating equation (2) we have

$$\begin{aligned} & M_y \frac{\partial v_r}{\partial r} + v_r \frac{\partial M_y}{\partial r} + \frac{M_y}{r} \frac{\partial v_\theta}{\partial \theta} + \frac{v_\theta}{r} \frac{\partial M_y}{\partial \theta} + \frac{\partial M_y}{\partial t} \\ &= D_r \frac{\partial^2 M_y}{\partial r^2} + \frac{\partial D_r}{\partial r} \frac{\partial M_y}{\partial r} + \frac{D_\theta}{r^2} \frac{\partial^2 M_y}{\partial \theta^2} \\ &+ \frac{1}{r^2} \frac{\partial D_\theta}{\partial \theta} \frac{\partial M_y}{\partial \theta} + \frac{F_o}{T_o} \gamma \beta_1(r, t) \end{aligned} \quad (3)$$

The transformation of equation (3) involves introducing a new variable by making some assumptions (Sprawls, 2000)

$$r = e^{u_0 R} \quad (3a)$$

and

$$\theta = e^{w_0 \theta} \quad (3b)$$

From (a) we have

$$\partial r = u_0 r \partial R$$

Also, from (b)

$$\left. \begin{aligned} \frac{\partial \theta}{\partial \theta} &= w_0 \theta \frac{\partial \theta}{\partial \theta} \\ \frac{\partial v_\theta}{\partial \theta} &= w_0 \\ \frac{\partial M_y}{\partial r} &= \frac{1}{u_0 r} \frac{\partial M_y}{\partial R} \\ \frac{\partial M_y}{\partial \theta} &= \frac{1}{w_0 \theta} \frac{\partial M_y}{\partial \theta} \\ \frac{\partial D_\theta}{\partial \theta} &= 2 D_0 w_0^2 \theta \\ \frac{\partial D_r}{\partial r} &= 3 D_0 u_0^2 r^2 \end{aligned} \right\} \quad (3c)$$

Equation (3) can also be rearrange as

$$\begin{aligned} & M_y \frac{\partial v_r}{\partial r} + \left(v_r - \frac{D_r}{\partial r} \right) \frac{\partial M_y}{\partial r} + \frac{M_y}{r} \frac{\partial v_\theta}{\partial \theta} + \\ & \left(\frac{v_\theta}{r} - \frac{1}{r^2} \frac{\partial D_\theta}{\partial \theta} \right) \frac{\partial M_y}{\partial \theta} + \frac{\partial M_y}{\partial t} = D_r \frac{\partial^2 M_y}{\partial r^2} + \\ & \frac{D_\theta}{r^2} \frac{\partial^2 M_y}{\partial \theta^2} + \frac{F_o}{T_o} \gamma \beta_1(r, t) \end{aligned} \quad (4)$$

Substitute (c) and $v_r = u_0 r, v_\theta = w_0 z, D_r = D_0 u_0^2 r^3, D_\theta = D_0 w_0^2 \theta^2$ into (4) we have

$$\begin{aligned} & M_y \left(u_0 + \frac{w_0}{r} \right) + (1 - 3 D_0 u_0 r) \frac{\partial M_y}{\partial R} + \left(\frac{1}{r} - \frac{2}{r^2} D_0 w_0 \right) \frac{\partial M_y}{\partial \theta} \\ &+ \frac{\partial M_y}{\partial t} = \frac{D_0 r}{r} \frac{\partial^2 M_y}{\partial R^2} + D_0 \frac{\partial^2 M_y}{\partial \theta^2} + \frac{F_o}{T_o} \gamma \beta_1(r, t) \end{aligned} \quad (5)$$

If we then make the assumption that

$$\frac{F_o}{T_o} \gamma \beta_1(r, t) = M_y \left(u_0 + \frac{w_0}{r} \right)$$

Awojoyogbe *et al.* 2010,

Then equation (5) becomes

$$\begin{aligned} (1 - 3D_o u_0 r) \frac{\partial M_y}{\partial R} + \left(\frac{1}{r} - \frac{2}{r^2} D_o w_0 \right) \frac{\partial M_y}{\partial \theta} + \frac{\partial M_y}{\partial t} \\ = \frac{D_o r}{r} \frac{\partial^2 M_y}{\partial R^2} + D_o \frac{\partial^2 M_y}{\partial \theta^2} \end{aligned} \quad (6)$$

equation (6) can also be written as

$$\begin{aligned} \frac{\partial M_y}{\partial t} = D_o \left(r \frac{\partial^2 M_y}{\partial R^2} + \frac{\partial^2 M_y}{\partial \theta^2} \right) - \\ (1 - 3D_o u_0 r) \frac{\partial M_y}{\partial R} - \left(\frac{1}{r} - \frac{2D_o w_0}{r^2} \right) \frac{\partial M_y}{\partial \theta} \end{aligned} \quad (7)$$

It is always possible to find solutions of the equation above, by separating into time and position coordinates. The method of the separation of variables relies upon the assumption that a function of the form $M_y = F(r, \theta) G(t)$

Where M_y is a function of r , θ and t , and F is a function of r , θ and G is a function of t alone, will be the solution to the partial differential equation above. Equation (7) can now be written as:

$$\begin{aligned} R \theta T' = D_o \left(r R'' \theta T + R \theta' T \right) \\ - (1 - 3D_o u_0 r) R' \theta T - \left(\frac{1}{r} - \frac{2D_o w_0}{r^2} \right) \theta' R T \end{aligned}$$

Divide through by $R \theta T$

$$\begin{aligned} \frac{T'}{T} = D_o \left(\frac{r R''}{R} + \frac{\theta'}{\theta} \right) \\ - (1 - 3D_o u_0 r) \frac{R'}{R} - \left(\frac{1}{r} - \frac{2D_o w_0}{r^2} \right) \frac{\theta'}{\theta} \end{aligned}$$

Equate both sides with a constant $-\lambda^2$ to have

$$\frac{T'}{T} = -\lambda^2 \quad (7)$$

$$\begin{aligned} D_o \left(\frac{r R''}{R} + \frac{\theta'}{\theta} \right) - (1 - 3D_o u_0 r) \frac{R'}{R} - \left(\frac{1}{r} - \frac{2D_o w_0}{r^2} \right) \frac{\theta'}{\theta} \\ = -\lambda^2 \end{aligned} \quad (8)$$

From (7),

$$T' + T \lambda^2 = 0 \quad (9)$$

Let

$$\left. \begin{aligned} T &= A e^{m t} \\ T' &= A m e^{m t} \end{aligned} \right\} \quad (10)$$

Putting (10) into (9)

$$A e^{m t} (m + \lambda^2) = 0$$

$$A e^{m t} \neq 0$$

$$m + \lambda^2 = 0$$

$$m = -\lambda^2$$

Therefore

$$T = A e^{-\lambda^2 t} \quad (11)$$

Also from (8)

$$\begin{aligned} D_o r \frac{R''}{R} - (1 - 3D_o u_0 r) \frac{R'}{R} + \lambda^2 \\ = -D_o \frac{\theta'}{\theta} + \left(\frac{1}{r} - \frac{2D_o w_0}{r^2} \right) \frac{\theta'}{\theta} \end{aligned} \quad (12)$$

Equation (12) can also be separated by equating both sides with a constant μ^2 and by re-arrangement we obtain

$$D_o r R'' - (1 - 3D_o u_0 r) R' + (\lambda^2 - \mu^2) R = 0 \quad (13)$$

$$-D_o \theta'' + \left(\frac{1}{r} - \frac{2D_o w_0}{r^2} \right) \theta' - \theta \mu^2 = 0 \quad (14)$$

Equation (14) can also be written as

$$D_o \theta'' - \left(\frac{1}{r} - \frac{2D_o w_0}{r^2} \right) \theta' + \theta \mu^2 = 0 \quad (15)$$

From (13)

$$\left. \begin{aligned} R &= A e^{m R} \\ R' &= A m e^{m R} \\ R'' &= A m^2 e^{m R} \end{aligned} \right\} \quad (16)$$

Substitute (16) into (13)

$$A e^{m R} \left[D_o r m^2 - (1 - 3D_o u_0 r) m + (\lambda^2 - \mu^2) \right] = 0$$

$$A e^{m R} \neq 0$$

$$D_o r m^2 - (1 - 3D_o u_0 r) m + (\lambda^2 - \mu^2) = 0$$

$$m = \frac{(1 - 3D_o u_0 r) \pm \sqrt{(1 - 3D_o u_0 r)^2 - 4D_o (\lambda^2 - \mu^2)}}{2D_o r}$$

Therefore,

$$R = A_1 e^{\frac{(1-3D_0u_0r) + \sqrt{(1-3D_0u_0r)^2 - 4D_0r(\lambda^2 - \mu^2)}}{2D_0r}} + A_2 e^{\frac{(1-3D_0u_0r) - \sqrt{(1-3D_0u_0r)^2 - 4D_0r(\lambda^2 - \mu^2)}}{2D_0r}} \quad (17)$$

From (17) let

$$(1-3D_0u_0r)^2 - 4D_0r(\lambda^2 - \mu^2) = \alpha$$

And making $A_1 = A_2$ we have:

$$R = e^{\frac{(1-3D_0u_0r)}{2D_0r}} A_1 \left[e^{\frac{\sqrt{\alpha}}{2D_0r} R} + e^{-\frac{\sqrt{\alpha}}{2D_0r} R} \right]$$

$$R = 2e^{\frac{(1-3D_0u_0r)}{2D_0r}} A_1 \left[\cosh \frac{\sqrt{\alpha}}{2D_0r} R \right]$$

$$\left. \begin{aligned} \theta &= Be^{m\theta} \\ \theta' &= Bme^{m\theta} \\ \theta'' &= Bme^{m\theta} \end{aligned} \right\} \quad (18)$$

Put (18) into (15)

$$Be^{m\theta} \left[D_0 m^2 - \left(\frac{1}{r} - \frac{2D_0w_0}{r^2} \right) m + \mu^2 \right] = 0$$

$$Be^{m\theta} \neq 0$$

$$D_0 m^2 - \left(\frac{1}{r} - \frac{2D_0w_0}{r^2} \right) m + \mu^2 = 0$$

$$m = \frac{\left(\frac{1}{r} - \frac{2D_0w_0}{r^2} \right) \pm \sqrt{\left(\frac{1}{r} - \frac{2D_0w_0}{r^2} \right)^2 - 4D_0\mu^2}}{2D_0}$$

Therefore,

$$\theta = B_1 e^{\frac{\left(\frac{1}{r} - \frac{2D_0w_0}{r^2} \right) + \sqrt{\left(\frac{1}{r} - \frac{2D_0w_0}{r^2} \right)^2 - 4D_0\mu^2}}{2D_0} \theta} + B_2 e^{\frac{\left(\frac{1}{r} - \frac{2D_0w_0}{r^2} \right) - \sqrt{\left(\frac{1}{r} - \frac{2D_0w_0}{r^2} \right)^2 - 4D_0\mu^2}}{2D_0} \theta} \quad (19)$$

$$\text{From (19), let } \left(\frac{1}{r} - \frac{2D_0w_0}{r^2} \right)^2 - 4D_0\mu^2 = \gamma$$

$$\theta = e^{\frac{\left(\frac{1}{r} - \frac{2D_0w_0}{r^2} \right)}{2D_0} \theta} \left[B_1 e^{\frac{\sqrt{\gamma}}{2D_0} \theta} + B_2 e^{-\frac{\sqrt{\gamma}}{2D_0} \theta} \right]$$

If we let $B_1 = B_2$ we have:

$$\theta = B_1 e^{\frac{(1-2D_0w_0)}{2D_0} \theta} \left[e^{\frac{\sqrt{\gamma}}{2D_0} \theta} + e^{-\frac{\sqrt{\gamma}}{2D_0} \theta} \right]$$

Then the transverse magnetization becomes

$$M_y = 4e^{\frac{(1-3D_0u_0)}{2D_0} R} A_1 \left[\cosh \frac{\sqrt{\alpha}}{2D_0} R \right] \cdot B_1 e^{\frac{(1-2D_0w_0)}{2D_0} Z} \left[\cosh \frac{\sqrt{\gamma}}{2D_0} Z \right] \cdot A e^{-\lambda^2 t} \quad (20)$$

The solution above is the NMR transverse magnetization and signal in spherical geometry. This NMR signal is a function of diffusion coefficient D_0 . The solution can be a tool to accurately understand the combined effect of diffusion and perfusion processes in human physiological and pathological flow systems. There seems to be evidence to suggest that in some transport processes the velocity and diffusion coefficients are not constants but functions of time and space (Zoppou and, Knight. 999).

3. Conclusions

We have obtained basic expression for the transverse magnetization (the NMR signals) in spherical geometry based on the Bloch NMR flow equations. This general solution is quite interesting and promising in the context of some recent research works on dynamical flow. The application of this fundamental solution to solve real life flow problems in which NMR-sensitive materials are transported will be presented separately.

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